

STIC Database Tracking Number: 305957

To: MATTHEW SUCH
Location: JEF-6B85
Art Unit: 2891
Tuesday, August 25, 2009

Case Serial Number: 10/576,914

From: SCOTT SEGAL
Location: EIC2800
JEF-4B55
Phone: (571)272-1314

scott.segal@uspto.gov

Search Notes

Re: Novel Diketopyrrolopyrrole Polymers

Examiner Such:

Attached are edited search results from the patent and NPL literature in STN. Chemical structure searching was conducted in CAS Registry and Chemical Abstracts. Please note that due to the amount of results, I had to split the pdf file into two separate files.

The **asterisked** items are some of the results worth your review. However, I recommend that you browse all the results.

If you would like more searching to be done on this case, or if you have questions or comments, please do not hesitate to contact me.

Respectfully,
Scott

Scott Segal
Searcher, STIC-EIC2800
JEF-4B55, 571-272-1314



AUG 20

3 65957

EIC 2800 SEARCH REQUEST

Today's Date 8/19/2009Name MATTHEW SUCHPriority App. Filing Date 10/18/2004AU/Org. 2891 Employee # 81973Case/App. # 10/576914JEF
Bld.&Rm.# 8B85 Phone 2-8895**Format for Search Results**EMAIL ☒PAPER ☐If this is an Appeals case, check here ☐

Describe this invention in your own words

PLEASE SEARCH ATTACHED POLYMER

Synonyms

THANKS!**Additional Comments**

Please submit completed form to your EIC.

STIC USE ONLY

Searcher

Scott Segal

Date Completed

8/25/09

Phone

2-1314

Sources

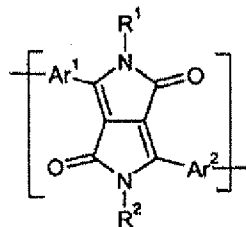
CAS Registry Chemical Abstracts

01/09

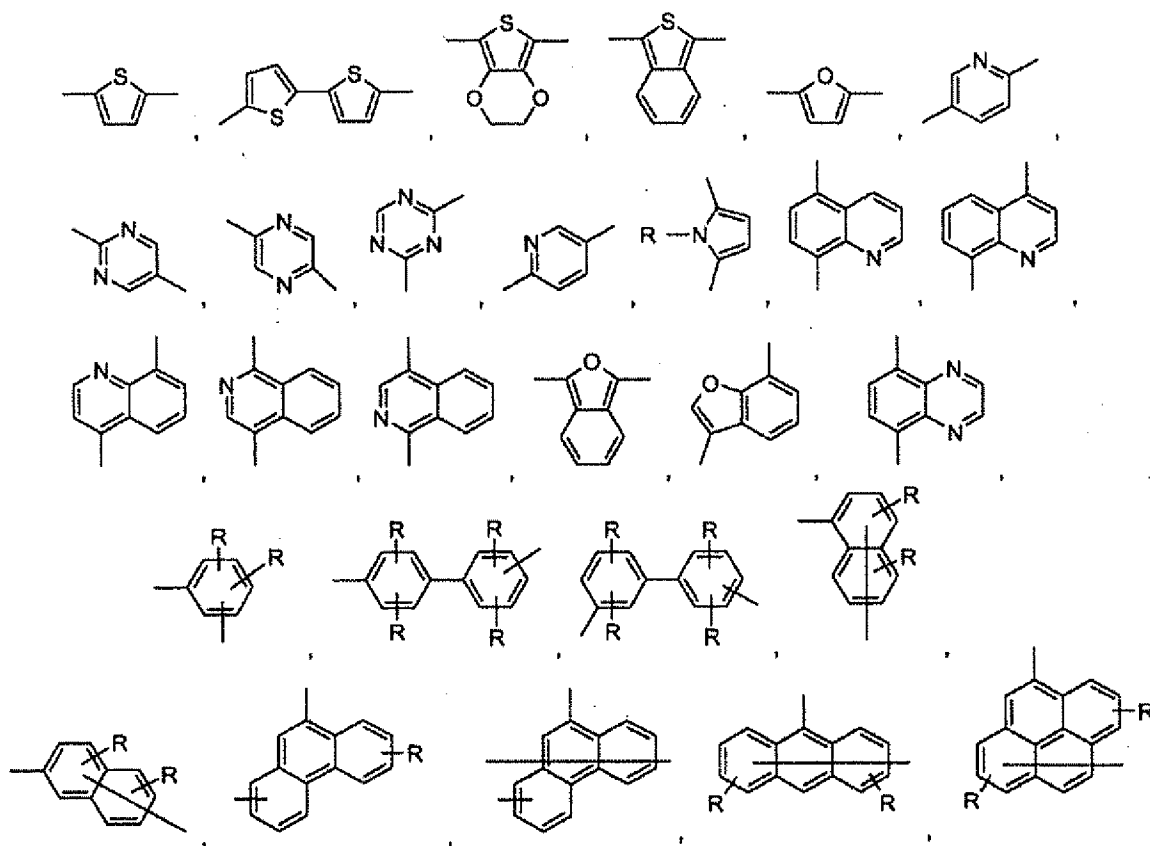
10/576914

DATE: 18 OCT. 2004

POLYMER OF:



wherein Ar¹ and Ar² are independently of each other



R can be anything, ie. C₁-C₂₅ alkyl



VOLUNTARY SEARCH FEEDBACK



Art Unit _____

App./Serial # _____

How did you use your search results?

You may cut and paste into the box below

☐ I02 rejection

☐ I03 rejection

☐ Cited in allowance

} Citations or
Patents Used

In brief - citation #, author, or patent #

☐ Helped better understand state of the art in technology, or specific invention

☐ Results verified the lack of relevant prior art (helped determine patentability).

Types ☐ Patent(s)

☐ Non-Patent Literature

COMMENTS

Questions about the scope or the results of the search?

Contact your EIC searcher or EIC Supervisor.

Please submit completed form to your EIC.

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Today's Date _____

Additional Notes if applicable (please indicate all actions including emails, phone calls, and individuals assisting):

10/576,914

8/25/09

STN

Search Histories

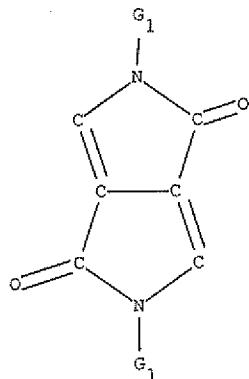
09:48:32 ON 25 AUG 2009

09:58:22 ON 25 AUG 2009

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L1 STRUCTURE UPLOADED

D L1



L2 30 SEA SSS SAM L1

L3 945 SEA SSS FUL L1

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L4 267 SEA ABB=ON L3

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L6 117 SEA ABB=ON L4 AND (?PYRROLO(5W)?PYRROLE?)

L7 174 SEA ABB=ON (L5 OR L6)

L8 22 SEA ABB=ON L7 AND ?THIOPHEN?

L9 44 SEA ABB=ON L7 AND (C08G61-12 OR C09K11-06 OR C09K11-06 OR C08G61-00 OR C08G73-00 OR C08G73-06 OR C09K11-00)/IPC,IC

L10 20 SEA ABB=ON L7 AND (H05B33-00 OR H05B33-02 OR H05B33-10 OR H05B33-14 OR H05B33-22 OR H05B33-28)/IPC,IC

L11 51 SEA ABB=ON L7 AND (CHEMILUMINESC? OR ?LUMINESC? OR ELECTROLUMINESC? OR CATHODOLUMINESC? OR BIOLUMINESC? OR ELECTROLUMINESC? OR FLUOROSCENC? OR SUPERFLUORESC? OR MAGNETOLUMINESC?)

L12 0 SEA ABB=ON L7 AND (ELECTROCHEMILUMINESCENCE)/CT

L13 39 SEA ABB=ON L7 AND (ELECTROLUMINESC#####)

L14 62 SEA ABB=ON L7 AND (?FLUORESC? OR ?PHOSPHORESC?)

L15 11 SEA ABB=ON L7 AND (LIGHT OR RADIAT##### OR IRRADIAT##### OR IRRAD## OR PHOTON) (2A) (EMIT##### OR EMISS##### OR DIFFUS##### OR PROPAGAT?)

L16 2 SEA ABB=ON L7 AND (SEMICONDUCT#####) (2A) (LASER OR LIGHT##### OR DIODE)

L17 0 SEA ABB=ON L7 AND (LIGHT EMIT#####) (1W) (SEMICONDUCTOR OR WAFER OR IC OR INTEGRATED CIRCUIT OR CHIP OR MICROCHIP OR CIRCUIT? OR DIE)

L18 7 SEA ABB=ON L7 AND (OLED OR LED OR PLED OR OEL)

L19 0 SEA ABB=ON L7 AND (ORGANIC LIGHT) (W) (EMIT? OR EMIS?)

L20 0 SEA ABB=ON L7 AND (TOLED OR SOLED OR SMOLED)

L21 1 SEA ABB=ON L7 AND (POLYMER LIGHT) (W) (EMIS? OR EMIT?)

L22 5 SEA ABB=ON L7 AND (ORGANIC OR POLYMER?) (3A) (EL OR LED OR LCD)

L23 19 SEA ABB=ON L7 AND (EMIS? OR EMIT? OR LED OR LCD) (5A) (ORGANIC OR POLYMER?)

L24 23 SEA ABB=ON L7 AND (EL OR ELECTROLUMIN?) (5A) (ORGANIC OR POLYMER? OR ELEMENT)

L25 1 SEA ABB=ON L7 AND (METAL OXIDE SEMICONDUCTOR FIELD EFFECT TRANSISTOR OR TFT OR ?MOSFET? OR MISFET OR MOS OR CMOS OR PMOS OR NMOS OR SBMOS OR LOCOS OR FET OR IGFET OR HMET OR HEMT OR OFET OR LDMOS)

L26 8 SEA ABB=ON L7 AND (FIELD EFFECT TRANSISTOR OR ?TRANSISTOR? OR JFET OR OTFT OR PFET OR NFET OR COMPLIMENTARY METAL OXIDE? OR BICMOS OR MESFET OR CHEMFET OR ISFET OR HFET OR IGBT OR MUGFET)

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L28 103 SEA ABB=ON (L8 OR L9 OR L10 OR L11 OR L12 OR L13 OR L14 OR L15 OR L16 OR L17 OR L18 OR L19 OR L20 OR L21 OR L22 OR L23 OR L24 OR L25 OR L26 OR L27)

L29 48 SEA ABB=ON L28 AND P/DT

L30 55 SEA ABB=ON L28 NOT L29

L31 28 SEA ABB=ON L30 NOT 2005-2009/PY
L32 36 SEA ABB=ON L29 AND 1980-2004/PRY,PY
L33 33 SEA ABB=ON L29 AND 2005-2009/PRY,PY
L34 15 SEA ABB=ON L29 NOT L33
L35 64 SEA ABB=ON L34 OR L32 OR L31
D HITSTR HITIND 8
D L35 IBIB ABS HITSTR HITIND 1-64

10/576,914

8/25/09

STN

08:33:46 ON 25 AUG 2009

09:14:54 ON 25 AUG 2009

FILE 'HCAPLUS' ENTERED AT 08:33:56 ON 25 AUG 2009

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E YU L, 1994, V115/RE

L2 26 SEA ABB=ON ("YU L, 1994, V116, P2647, J AM CHEM SOC"/RE OR
"YU L, 1994, V116, P9733, J AM CHEM SOC"/RE OR "YU L, 1994,
V116, P9733, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY"/RE)
E YU L, 1993, VOL34/RE
E LUPING T, 1994, V64/RE
E LUPING Y, 1994, VOL64/RE
E LUPING Y, 1994, V64/RE
E LUPING Y, 1994/RE
E YU L, 1994, V64/RE

L3 42 SEA ABB=ON ("YU L, 1994, V64, P2489, APPL PHYS LETT"/RE OR
"YU L, 1994, V64, P2489, APPLIED PHYSICS LETTERS"/RE OR "YU L,
1994, V64, P536, APPL PHYS LETT"/RE OR "YU L, 1994, V64, P9,
APPL PHYS LETT"/RE OR "YU L, 1994, V64, PPP2489, APPL PHYS LETT"/RE)

L4 2 SEA ABB=ON (EXPLORATION)/TI AND (STILLE COUPLING)/TI
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L5 169 SEA ABB=ON ("BAO Z, 1995, V117, P12426, J AM CHEM SOC"/RE OR
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1995, V117, P12426, JOURN AM CHEM SOC"/RE OR "BAO Z, 1995,
V117, P12426, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY"/RE OR
"BAO Z, 1995, V117, P12427, J AM CHEM SOC"/RE)
E HORN M, 2002/RE
E HORN M, 2002, V117/RE
E HORN M, 2002, V38/RE

L6 7 SEA ABB=ON ("HORN M, 2002, V38, P2197, EUR POLYM J"/RE OR
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E EP1078970/RE
E TIEKE B, 2001/RE
E EP1078970/PN

L7 1 SEA ABB=ON EP1078970/PN
E EP1078970/RE
E 1078970/RE

L8 242 SEA ABB=ON L2 OR L3 OR L5 OR L6

L9 2 SEA ABB=ON L8 AND P/DT

L10 240 SEA ABB=ON L8 NOT L9

L11 167 SEA ABB=ON L10 NOT 2005-2009/PY

L12 169 SEA ABB=ON L9 OR L11

L13 5 SEA ABB=ON L12 AND (?PYRROLOPYRROLE? OR PYRROLO PYRROLE?)
D IBIB ABS 1-5
E PRAEFCKE K, 1998/RE

L14 6 SEA ABB=ON "PRAEFCKE K, 1998, V24, P153, LIQ CRYST"/RE
E ALP S, 2003/RE

L15 2 SEA ABB=ON ("ALP S, 2004, V60, P103, DYES PIGM"/RE OR "ALP S,
2004, V60, P103, DYES PIGMENTS"/RE)

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D ALL 1-2

FILE 'PCI' ENTERED AT 09:04:15 ON 25 AUG 2009

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L19 4 SEA ABB=ON EP1078970/PN.D
E US6451459/PN.D

L20 6 SEA ABB=ON US6451459/PN.D

L21 8 SEA ABB=ON (L19 OR L20)

L22 SEL L21 1- PRN : 9 TERMS

FILE 'HCAPLUS, WPIX' ENTERED AT 09:05:17 ON 25 AUG 2009

L23 14 SEA ABB=ON L22

L24 14 SEA ABB=ON L23 AND F/DT

L25 12 SEA ABB=ON L24 AND 1980-2004/PRY, PY

L26 12 SEA ABB=ON L24 AND 2005-2009/PRY, PY

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L28 12 SEA ABB=ON L27 OR L26
D IBIB ABS TI 1-12



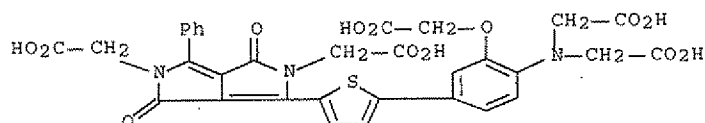
L35 ANSWER 11 OF 64 COPYRIGHT ACS on STN
 ACCESSION NUMBER: 2004:785421 HCAPLUS
 TITLE: Synthesis and in vitro evaluation of
dioxopyrrolopyrroles as potential low-affinity
fluorescent Ca²⁺ indicators
 AUTHOR(S): Avciyasi, Nesibe; Smet, Mario; Metten, Bert; Dehaen,
 Wim; de Schryver, Frans C.; Bultynck, Geert;
 Callewaert, Geert; de Smedt, Humbert; Missiaen,
 Ludwig; Boens, Noel
 CORPORATE SOURCE: Department of Chemistry, Katholieke Universiteit
 Leuven, Heverlee, 3001, Belg.
 SOURCE: International Journal of Photoenergy (2004), 6(4),
 159-167
 PUBLISHER: Ain Shams University, Photoenergy Center
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Three new low-affinity **fluorescent** Ca²⁺ indicators excitable with visible
 light, 3-phenyl-6-(4-(3-carboxymethoxy-4-(N,N-
 dicarboxymethylamino)phenyl)phenyl)-2,5-dicarboxymethyl-1,4-
dihydropyrrolo[3,4-c]**pyrrole**-1,4-dione (DPP1), 3-phenyl-6-(5-(3-carboxymethoxy-
 4-(N,N-dicarboxymethyl-amino)phenyl)thien-2-yl)-2,5-dicarboxymethyl-1,4-
dihydropyrrolo[3,4-c]**pyrrole**-1,4-dione (DPP2) and
 3-(thien-2-yl)-6-(5-(3-carboxymethoxy-4-(N,N-
 dicarboxymethylamino)phenyl)thien-2-yl)-2,5-dicarboxymethyl-1,4-
dihydropyrrolo[3,4-c]**pyrrole**-1,4-dione (DPP3) were synthesized and evaluated
 for their Ca²⁺ binding properties via fluorometric titrns. The in vitro
 dissociation constant K_d measured at 21° in 100 mM KCl buffered solution, pH
 7.05, for the Ca²⁺-DPP1 complex is 10 μM; for Ca²⁺-DPP2 and Ca²⁺-DPP3 a K_d
 value of 20 μM is found. All three indicators form 1: 1 complexes with Ca²⁺.
 The **fluorescence** quantum yields of the uncomplexed forms of DPP1, DPP2 and DPP3
 are 1.2 + 10⁻², 3.4 + 10⁻² and 3.6 + 10⁻², resp. After binding to Ca²⁺ these
 values increase to 4.8 + 10⁻², 5.0 + 10⁻² and 5.1 + 10⁻², resp.

IT 853415-45-9P 853415-46-0P 853415-47-1P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (synthesis and in vitro evaluation of **dioxopyrrolopyrroles** as
 potential low-affinity **fluorescent** Ca²⁺ indicators)

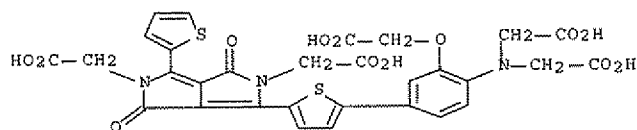
RN 853415-46-0 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-2,5(1H,4H)-diacetic acid,
 3-[5-[4-[bis(carboxymethyl)amino]-3-(carboxymethoxy)phenyl]-2-thienyl]-1,4-
 dioxo-6-phenyl- (CA INDEX NAME)



RN 853415-47-1 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-2,5(1H,4H)-diacetic acid,
 3-[5-[4-[bis(carboxymethyl)amino]-3-(carboxymethoxy)phenyl]-2-thienyl]-1,4-
 dioxo-6-(2-thienyl)- (CA INDEX NAME)





Handwritten mark

(12) **EUROPEAN PATENT APPLICATION**

(43) Date of publication:
28.02.2001 Bulletin 2001/09

(51) Int Cl.7: **C09K 11/06, C08C
H05B 33/14**

*Same Assignee
as 10/576, 914*

(21) Application number: **00810727.8**

(22) Date of filing: **16.08.2000**

(84) Designated Contracting States:
**AT BE CH CY DE DK ES FI FR GB GR IE IT LI LU
MC NL PT SE**
Designated Extension States:
AL LT LV MK RO SI

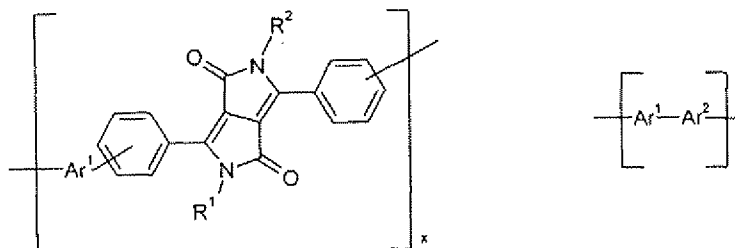
(72) Inventors:
• **Tieke, Bernd**
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• **Beyerlein, Thomas**
50737 Köln (DE)
• **Brütting, Wolfgang**
91344 Waischenfeld (DE)
• **Forero-Lenger, Stefan**
95448 Bayreuth (DE)

(30) Priority: **26.08.1999 EP 99810773**

(71) Applicant: **Ciba Specialty Chemicals Holding Inc.**
4057 Basel (CH)

(54) **DPP-containing conjugated polymers and electroluminescent devices**

(57) diketopyrrolopyrrole (DPP) based polymers and copolymers comprising the following units



wherein x is chosen in the range of from 0.005 to 1, and y from 0.995 to 0, and wherein $x + y = 1$, and wherein Ar^1 and Ar^2 independently from each other stand for



(10) Patent No.: US 6,451,459 B1
(45) Date of Patent: Sep. 17, 2002

(57) **ABSTRACT**
Diketopyrrolopyrrole (DPP) based polymers comprising the following units

Same Assignee
as 10/57, 914

$$\left[\text{Ar}' - \text{C}_6\text{H}_4 - \text{C}(\text{N}^{\text{R}^1})=\text{C}(\text{N}^{\text{R}^2})=\text{C}(\text{CH}_3)_2 \right]_n$$

(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 131 days.

wherein x is chosen in the range of from 0.005 to 1, and y from 0.995 to 0, and wherein $x+y=1$, and wherein Ar^1 and Ar^2 independently from each other stand for

(30) Foreign Application Priority Data

Aug. 26, 1999 (EP) 99810773

(51) **Int. Cl.⁷** **H05B 33/14; C08G 61/12;**
C09K 11/06

(52) U.S. Cl. 428/690; 428/917; 313/504;
313/506; 257/40; 252/301.35; 528/367;
528/394; 528/397

(58) **Field of Search** 428/690, 917;
313/504, 506; 257/40; 252/301.35; 528/367,
394, 397

(56) **References Cited**

U.S. PATENT DOCUMENTS

5.750.723 A 5/1998 Eldin et al. 548/453

FOREIGN PATENT DOCUMENTS

EP	0 499 011	8/1992
EP	0 787 730	8/1997

OTHER PUBLICATIONS

T. Beyerlein et al., "New photoluminescent conjugated polymers with . . . (DPP) and 1,4-phenylene units . . .", *Macromol. Rapid Commun.* 21(4), pp. 182-189 (2000).
J. of Amer. Chem. Soc. vol. 115, pp. 11735-11743 (1993).
no month.
J. of Amer. Chem. Soc. vol. 117, pp. 12426-12435 (1995).
no month.
Appl. Phys. Letters vol. 64, pp. 2489-2491 (May 1994).
Macromol. Chem. Phys. vol. 200, pp. 106-112, (1999).
no month.

* cited by examiner

Primary Examiner—Marie Yamnitzky
(74) *Attorney, Agent, or Firm*—David R. Crichton

9 Claims, No Drawings

Full-text
included

*

Novel family of liquid crystals based on a known pigment material: mesomorphic derivatives of 2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione†

by KLAUS PRAEFCKE*, MARKUS JACHMANN, DIRK BLUNK
and MATTHIAS HORN

Institute of Organic Chemistry, Technische Universität Berlin, D-10623 Berlin,
Germany

*Presented at the Capri Symposium in Honour of George W. Gray, FRS held at the
Hotel Palatium, Capri, 11-14 September 1996*

The chromophoric biheterocycle 2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (DPPD) as a widely variable basic core structure has been introduced into liquid crystal research and the first eight calamitic examples of thermomesomorphic derivatives are presented and discussed.

1. Introduction

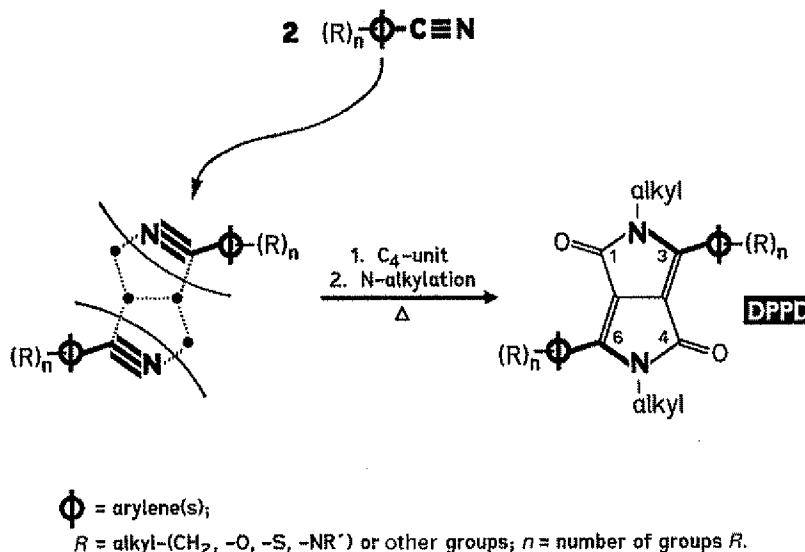
Derivatives of the 3,6-diaryl-substituted biheterocyclic compound 2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (DPPD, figure 1) constitute a relatively new class of chemically stable fluorescent molecules of which the first examples were synthesized as long as 22 years ago [2]; however, most work with them dates only from recent years [3-9].

Although in the course of this activity DPPDs were studied from various scientific and technological aspects, e.g. their applications as photostable and weatherproof pigments—orange, red, or red-violet, etc. in colour—

laser, safety, and textile dyes, fluorescence dyes with large Stokes shifts, photosensitizers, or materials for the storage of digital data, etc. surprisingly thus far no reports regarding the relationship between low molar mass DPPDs and liquid crystalline properties are available in the literature.

The only connections of DPPDs with liquid crystals which have come to our knowledge are given in the references [7-9] dealing with (1) rational designs of multifunctional liquid crystalline conjugated polymers containing a *non-thermomesomorphic* DPPD derivative as photosensitizer [7,9] and (2) polarized light spectro-

Figure 1. Sketch of the two-step synthetic route to the tetrasubstituted 2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-diones (DPPD) from arynitriles and a C₄-unit (e.g. dialkyl succinates) on heating with base induction, followed by a classical N-alkylation reaction. This chromophoric biheterocycle is introduced here as a new core system in liquid crystal research.



*Author for correspondence.

†See reference [1].

scopy of DPPDs with small substituents in an anisotropic environment, i.e. as additives in a macroscopically aligned lyotropic nematic liquid crystal [8].

In our opinion, the reason for this gap regarding this relationship between DPPD compounds and their mesomorphic behaviour lies clearly in the kind of substitution used in the aryl nitrile, the main starting material for the 3,6-diaryl DPPD derivatives (figure 1), hitherto characterized by only *short* substituents due to other interests (see above) in this fascinating chromophoric system.

2. Experimental

2.1. General

The chemical structures of all final products were confirmed by standard methods: elemental analyses, NMR spectroscopy (400 MHz, solvent: CDCl_3), as well

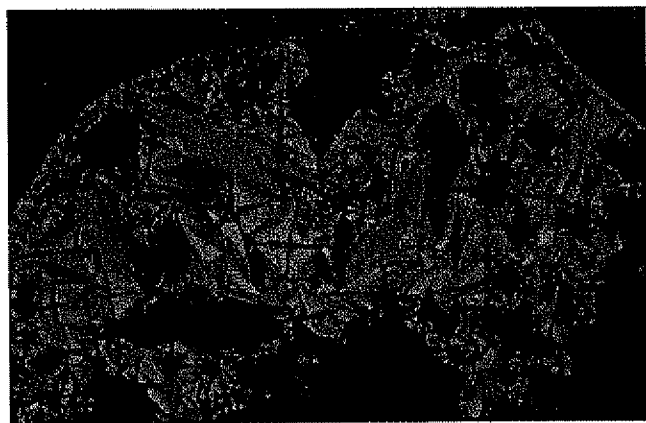
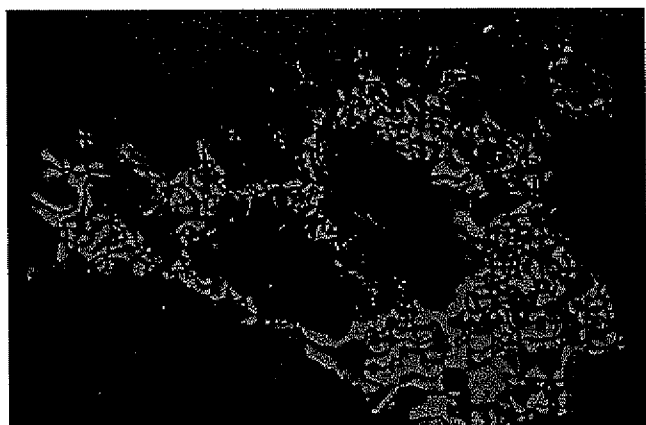


Figure 2. Characteristic textures of two examples of light red calamitic liquid crystals possessing the DPPD core shown in the table and figure 1: the schlieren texture (nematic, N phase between lipophilic glass plates: top) of **1a** at 113.3°C on heating into the isotropic liquid phase and the fan-like texture (smectic, SmA phase: bottom) of **1b** at 107.9°C on cooling from the isotropic liquid phase; heating or cooling rates 1 K min^{-1} .

as mass spectrometry (Varian MAT 711, 70 eV, $>200^\circ\text{C}$, direct inlet).

Instruments for further studies and calculations included (1) Optical microscopy: Leitz Laborlux 12 Pol with a Mettler FP82 microfurnace and a FP80 control unit; (2) DSC: Mettler TA 3000/DSC-30 S with TA 72.5 software; (3) X-ray: Cu-K_α radiation, beam width 0.4 mm, sealed capillary; (4) semi-empirical calculations: MNDO94 3.0/AM1 procedure, standard parameter set of the Unichem 3.0 software package (Cray Research Inc.), Cray J 932/16-8192 computer, SCF field consistency achieved.

2.2. Preparation of the DPPD derivatives **1a–h**

Starting from each 25 mmol of the respective aryl nitrile [10], the preparations of the red intermediate biheterocyclic product (yields: 12–35%) were carried out analogously to earlier descriptions [3]. Following an earlier procedure [3] for *N*-alkylations of analogous bis-lactams our preparations of **1a–h** ($\leq 50\%$ yield) were made on a 2 mmol scale. The phase transition data and types of mesophase are listed in the table; two texture photographs are shown in figure 2. Satisfactory elemental analyses and spectroscopic data for **1a–h** were obtained.

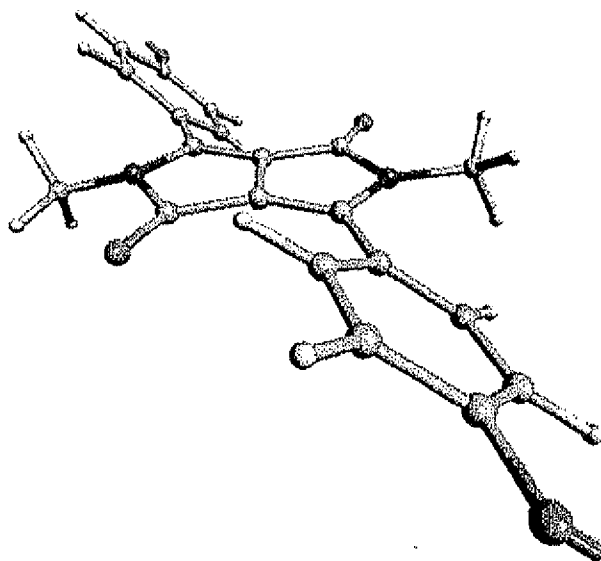


Figure 3. The ball-and-stick model of the new, light red DPPD liquid crystal **1c** [3,6-bis(4'-dodecyloxyphenyl)-2,5-dihydro-*N,N'*-dimethylpyrrolo[3,4-*c*]pyrrole-1,4-dione] (table), used here as an example from the 3,6-diaryl DPPD series to demonstrate the angle between the biheterocyclic molecular centre unit and the phenyl substituents attached to it; this was calculated (cf. §2.1) by us semi-empirically to be 30–40°. In its fully stretched form **1c** is about 43.6 Å long and 6.1 Å wide. However, to enable concentration on the angle situation in the model shown, the chains have been omitted.

The formulae and molar masses of the eight new *N,N'*-dialkylated thermotropic liquid crystal materials are:

1a C ₃₆ H ₄₈ N ₂ O ₄ (572.8),	1b C ₄₀ H ₅₆ N ₂ O ₄ (628.9),
1c C ₄₄ H ₆₄ N ₂ O ₄ (685.0),	1d C ₄₄ H ₄₈ N ₂ O ₄ (668.9),
1e C ₄₀ H ₄₀ N ₂ O ₂ (580.8),	1f C ₃₈ H ₄₈ N ₂ O ₂ (568.1),
1g C ₅₄ H ₆₄ N ₂ O ₂ (773.1),	1h C ₅₆ H ₆₈ N ₂ O ₂ (801.2).

3. Results and discussion

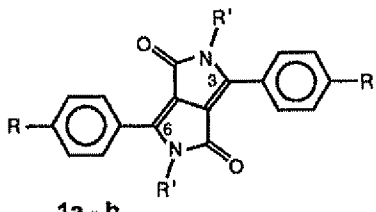
In an effort to test the suitability of the DPPD biheterocycle (see the structural formulae in the table and figure 1) as a liquid crystal core, we have begun work on this topic by synthesizing the eight bis-lactams **1a–h** starting from various 4-arylnitriles [10] with longer alkyl or alkoxy chains in their *para*-positions and diethyl succinate according to the literature [3], cf. §2. As expected, in comparison with other derivatives of this class of compounds [3, 5], the intermediate crude, as yet not *N*-alkylated products of cyclization

are extremely high melting, deep red solids. Their *N*-alkylation led to the new target compounds **1a–h** which crystallize in needles, are now light red in colour, have very much lower melting points than their precursors, and are indeed thermomesomorphic (table and figure 2).








Preliminary investigations of these first DPPD liquid crystal materials **1a–h** by three methods (optical microscopy, DSC and in part also X-ray diffraction) prove that they are always *mono*-thermomesomorphic and exhibit in six cases (**1a**, **1d–h**) a nematic phase and in the two cases **1b** and **1c** (carrying the longest alkoxy substituents) each a smectic A phase. Figure 2 depicts texture photographs of both types of mesophase observed so far with this new family of liquid crystal materials which, incidentally, have a distinct tendency for homeotropic alignment.

Whereas the group of three 3,6-diphenyl DPPD materials, **1a–c**, exhibit only narrow mesophases slightly above 100°C, the nematic phases of all the other five mesogens, **1d–h**, having two or even three—in part

Table. Phase transition temperatures* (°C) and enthalpies (ΔH in kJ mol⁻¹) for the first eight DPPD liquid crystal (LC) materials **1a–h**, light red in colour, synthesized in our laboratory.



1a–h

DPPD LC	R	R'	Cr		M		Iso
1a	H ₁₇ C ₈ O—	CH ₃	•	106.2/105.7 (59.2)	N	114.0/113.7 (0.9)	•
1b	H ₂₁ C ₁₀ O—	CH ₃	•	106.3/105.5 (68.9)	SmA	119.0/117.9 (3.0)	•
1c	H ₂₅ C ₁₂ O—	CH ₃	•	108.8/108.1 (81.9)	SmA	122.7/121.6 (4.7)	•
1d	H ₁₃ C ₆ O— 	CH ₃	•	205.0/204.5 (44.3)	N	335.0/336.7 (1.2)	•
1e	H ₉ C ₄ — 	CH ₃	•	220.0/219.0 (4.2)	N	330.0/331.3 (0.1)	•
1f	H ₇ C ₃ — 	CH ₃	•	191.0/189.8 (23.3)	N	358.0/356.2 (1.7)	•
1g	H ₁₁ C ₅ —  — 	CH ₃	•	248.5/248.5 (31.3)	N	327.0/327.3 (0.3)	•
1h	H ₁₁ C ₅ —  — 	C ₂ H ₅	•	244.1/242.2 (37.7)	N	349.4/347.1 (0.2)	•

* Obtained by polarizing microscopy/DSC; Cr=crystalline, M=mesophase, N=nematic, SmA=smectic A, I=isotropic liquid.

aromatic—six membered rings in line at both positions 3- and 6-, prolonging the conjugation with the two double bonds of the DPPD core, are very much more stable. They appear mostly above 200°C and persist up to a clearing temperature close to 360°C (table).

Concerning the conjugation in **1a–h**, our semi-empirical calculations of the conformation in the 3,6-diphenyl DPPD part of the molecules (cf. the ball-and-stick model in figure 3) resulted in an energy minimum for an angle of 30–40° between the phenyl rings and the DPPD core.

Mesogen **1a** shows in an X-ray beam diffuse first order reflections which, however, are of greater sharpness than expected for typical nematic phases and seem to suggest a tendency to form a layered structure, found to be characteristic for the homologues **1b** and **1c**. The layer spacings for the latter two materials were found to be 32.06 and 35.42 Å, respectively.

The strong tendency to form ordered molecular structures is also reflected during the crystallization processes of all members of series **1**, as their melting points could be supercooled only by several degrees during cooling at a rate of 1 K min⁻¹ from their mesophases. The needle-like crystals are formed so quickly that the preparations crystallize entirely in less than 1 min. Interestingly, the melting points of **1a–c** are hardly different, whereas their clearing points go up steeply by about 9 K between **1a** and **1c** (table).

4. Conclusion

Certainly, the diverse possibilities of substitution of this interesting chromophoric DPPD system, offered in principle through the aromatic groups at positions 3 and 6 and the two lactam functions, indicate great promise for future development of not only further

coloured calamitic mesogens, but presumably also coloured phasmodic, disc-like, and polymer liquid crystal materials.

We thank Dr E. Poetsch, E. Merck, Darmstadt, Germany, for chemicals and the Deutsche Forschungsgemeinschaft, Bonn, Germany, the European Union, Brussels, Belgium, and the Gesellschaft von Freunden der Technischen Universität Berlin for financial support of our liquid crystal research work.

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10/576,914

8/25/09

STN

Same Assignee
as 10/576/14

L35 ANSWER 8 OF 64 COPYRIGHT ACS on STN

ACCESSION NUMBER: 2004:872828 HCAPLUS

DOCUMENT NUMBER: 141:351424

TITLE: **Fluorescent diketopyrrolopyrroles**

INVENTOR(S): Yamamoto, Hiroshi; Dan, Norihisa

PATENT ASSIGNEE(S): **Ciba Specialty Chemicals Holding Inc., Switz.**

SOURCE: PCT Int. Appl., 83 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004090046	A1	20041021	WO 2004-EP50403	20040401 <--
EP 1611207	A1	20060104	EP 2004-725051	20040401 <--
CN 1771298	A	20060510	CN 2004-80009420	20040401 <--
JP 2006524281	T	20061026	JP 2006-505506	20040401 <--
KR 2006002963	A	20060109	KR 2005-719176	20051007 <--
MX 2005010866	A	20060605	MX 2005-10866	20051010 <--
IN 2005CN02934	A	20070608	IN 2005-CN2934	20051109 <--
US 20070010672	A1	20070111	US 2006-551976	20060713 <--
US 7501076	B2	20090310		
US 20090173916	A1	20090709	US 2009-319937	20090114 <--

PRIORITY APPLN. INFO.:

EP 2003-100972	A	20030410 <--
WO 2004-EP50403	W	20040401 <--
US 2006-551976	A3	20060713

AB **Fluorescent diketopyrrolopyrroles I** [R1, R2 = (halo-substituted) C1-25 alkyl, (C1-4 alkyl-substituted) allyl, cycloalkyl, (substituted) phenyl-cycloalkyl condensed group, alkenyl, cycloalkenyl, alkynyl, haloalkyl, haloalkenyl, haloalkynyl, ketone or aldehyde group, ester group, carbamoyl, silyl group, siloxanyl, (substituted) aryl, (substituted) heteroaryl, or CR3R4(CH2)mA3; m = 0-4; R3, R4 = H, C2-4 alkyl, or (substituted) Ph; A1, A1 = 5- or 6-membered heterocyclic ring containing 1-3 heteroatoms selected from N, O, and S] are prepared for use as guest and host chromophores in **electroluminescent** compns., with the absorption spectrum of the guest chromophore overlapping the **fluorescent** emission spectrum of the host chromophore and the **photoluminescence** emission peak of the host chromophore being 500-720 nm. A typical I was manufactured by reaction of 27.7 g 5-bromo-2-cyanopyridine 20 h at 100-110° with 16.2 g diisopropyl succinate in tert-amyl alc., and reaction of 2 g intermediate 21 h with 2.4 g BuI in NMP in the presence of tert.-BuOK.

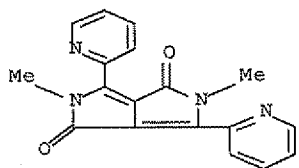
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 777079-62-6P 777079-63-7P 777079-64-8P
 777079-65-9P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(fluorescent diketopyrrolopyrroles for
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 absorption spectra overlapping host fluorescent emission
 spectra)

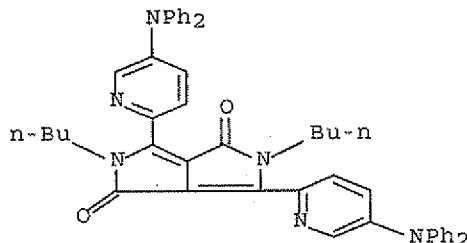
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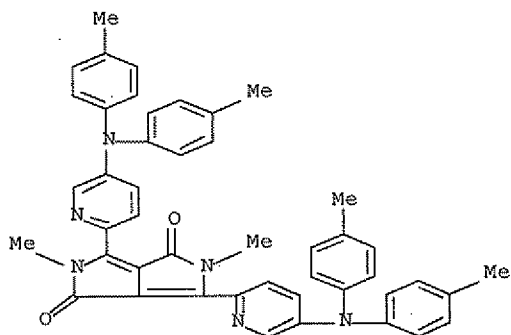
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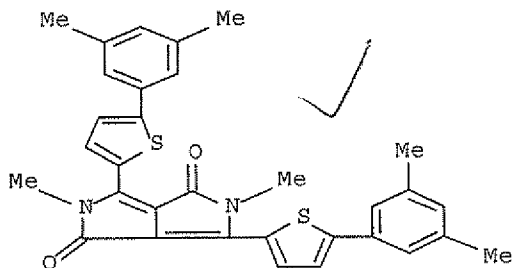
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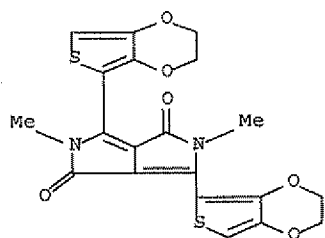
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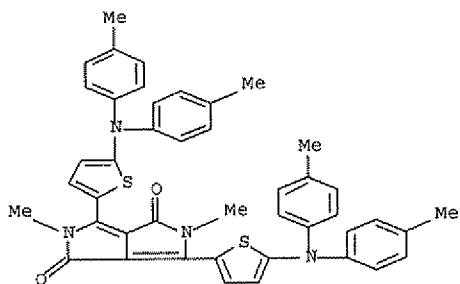


RN 777079-60-4 HCAPLUS

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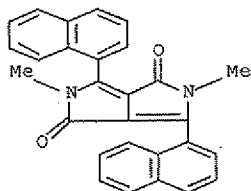


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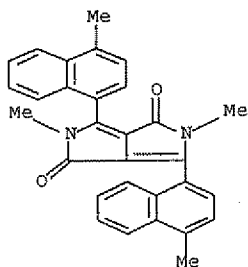


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 RL: TEM (Technical or engineered material use); USES (Uses)
 (host chromophore; **fluorescent diketopyrrolopyrroles**
 for **electroluminescent** compns. based on guest chromophores
 having absorption spectra overlapping host **fluorescent**
 emission spectra)

RN 474067-56-6 HCAPLUS
 CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dihydro-2,5-dimethyl-3,6-di-1-naphthalenyl- (CA INDEX NAME)



RN 777079-67-1 HCAPLUS
 CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dihydro-2,5-dimethyl-3,6-bis(4-methyl-1-naphthalenyl)- (CA INDEX NAME)



IT **Electroluminescent devices**
 (fluorescent diketopyrrolopyrroles for
electroluminescent compns. based on guest chromophores having
 absorption spectra overlapping host **fluorescent** emission
 spectra for devices)

10/576,914

8/25/09

STN

L35 ANSWER 19 OF 64 COPYRIGHT ACS on STN
ACCESSION NUMBER: 2003:792202 HCAPLUS
DOCUMENT NUMBER: 140:272320
TITLE: Photostability studies of thermomesomorphic
derivatives of 2,5-dihydropyrrolo[3,4-c]
pyrrole-1,4-dione
AUTHOR(S): Alp, Serap; Ertekin, Kadriye; Horn, Matthias; Icli,
Siddik
CORPORATE SOURCE: Faculty of Science and Arts, Department of Chemistry,
University of Dokuz Eylul, Izmir, Turk.
SOURCE: Dyes and Pigments (2003), Volume Date 2004, 60(2),
103-110
CODEN: DYPIDX; ISSN: 0143-7208
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In this study, the photophys. characteristics, like molar extinction coeffs.,
Stoke's shifts, quantum yields, radiative and **fluorescence** lifetimes,
fluorescence rate consts., radiationless deactivation rate consts., and singlet
energies of the **fluorescent** mesomorphic **diketopyrrolopyrrole** derivs., (DPPDs),
3,6-bis(4-octyloxyphenyl)-2,5-dihydro-2,5-dimethylpyrrolo [3,4-c]pyrrole-1,4-
dione and
3,6-bis(4'-butyl-4-biphenyl)-2,5-dihydro-2,5-dimethylpyrrolo [3,4-c]pyrrole-
1,4-dione have been determined. The photostability studies were carried out
under xenon arc lamp, direct and concentrated sunlight in solution of
chloroform and THF as well as in solid state, embedded in matrixes of
poly(vinyl chloride) (PVC) and TEOS sol-gel. The studies reveal that the
photostabilities of the DPPD derivs. in PVC and sol-gel matrixes are enhanced
compared to solns. of chloroform and THF.

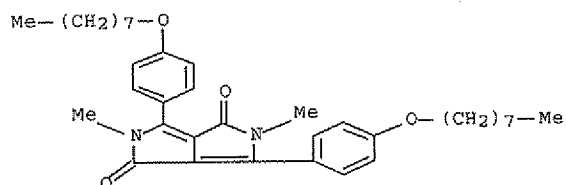
IT 205104-10-5 205104-14-9

RL: PRP (Properties); TEM (Technical or engineered material use); USES
(Uses)

(red pigment; photostability studies of thermomesomorphic derivs. of
dihydropyrrolopyrroledione pigments)

RN 205104-10-5 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dihydro-2,5-dimethyl-3,6-bis[4-
(octyloxy)phenyl]- (CA INDEX NAME)



CC 41-5 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic
Sensitizers)

Section cross-reference(s): 37, 73

ST **pyrrolopyrroledione** pigment photostability

IT **Fluorescence**

Sol-gel processing

(in photostability studies of thermomesomorphic derivs. of
dihydropyrrolopyrroledione pigments)

IT Photolysis

(solar; photostability studies of thermomesomorphic derivs. of
dihydropyrrolopyrroledione pigments)



Synthesis and characterisation of thermomesogenic polysiloxanes with 2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione units in the main chain

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Abstract

The synthesis of the first two liquid crystalline polysiloxanes bearing 3,6-diaryl-2,5-dihydropyrrolo-[3,4-c]pyrrole-1,4-dione units in their main chain are described. Investigations on their thermotropic phase behaviour by polarising microscopy reveal nematic or smectic enantiotropic phases, respectively.

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Keywords: Polysiloxanes; Liquid crystals; Diketopyrrolopyrrole

1. Introduction

Derivatives of 3,6-diaryl-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-diones (DPPD) represent relatively new members of the class of high performance pigments [1]. Due to their excellent all-round fastness properties this organic chromophore has been commercialised, e.g. in automotive paints and construction plastics and as well used for laser-, fluorescence dyes with large Stokes shifts or materials for the storage of digital data [2]. So far only a few reports on DPPD containing polymers and their materials properties are available in literature [3–8]. First, Yu and co-workers [4] reported the preparation of

a conjugated photorefractive polymer bearing a DPPD chromophore in its backbone by Stille coupling. Recently, two different series of deeply coloured and fluorescent polymers have been synthesised. Thus, copolyesters and urethanes with DPPD units in the main chain have been prepared. The chromophoric units have been incorporated in the backbone via their *N*-alkylated lactam groups [5]. The same research group also reported a different synthetic approach, using Suzuki coupling to introduce DPPD cores into π -conjugated polymers and co-polymers [6] in order to enhance the photoelectroluminescent [7,8] properties of this kind of macromolecules. Dehaen and co-workers [9] used Suzuki coupling in a stepwise sequence to obtain diketopyrrolopyrrole oligomers of well-defined length. To our knowledge, up to now, no reports regarding high molecular weight liquid crystalline DPPDs can be found in the literature.

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(19) **United States**(12) **Patent Application Publication** (10) Pub. No.: **US 2005/0008892 A1**
Yamamoto et al. (43) Pub. Date: **Jan. 13, 2005**(54) **FLUORESCENT COMPOSITIONS
COMPRISING
DIKETOPYRROLOPYRROLES**(76) Inventors: **Hiroshi Yamamoto, Nishinomiya-shi
(JP); Norihisa Dan, Yawata-shi (JP)**

Correspondence Address:
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CORPORATION
PATENT DEPARTMENT
540 WHITE PLAINS RD
P O BOX 2005
TARRYTOWN, NY 10591-9005 (US)**

(21) Appl. No.: **10/501,573**(22) PCT Filed: **Jan. 23, 2003**(86) PCT No.: **PCT/EP03/00650**(30) **Foreign Application Priority Data**

Feb. 1, 2002 (EP)..... 0245067.6
Sep. 12, 2002 (EP)..... 0245796.0

Publication Classification(51) Int. Cl.⁷ **C09K 11/**(52) U.S. Cl. **428/690; 428/
313/504; 3**(57) **ABSTRACT**

The present invention relates to composition comprising a guest chromophore and a host chromophore, wherein the absorption spectrum of the guest chromophore overlaps with the fluorescence emission spectrum of the host chromophore, wherein the host chromophore is a diketopyrrolopyrrole having an absorption peak at 500 to 720 nm, preferably 500 to 600 nm, most preferred 520 to 580 nm and wherein the guest chromophore is a diketopyrrolopyrrole having an absorption peak at 500 to 720 nm, preferably 500 to 600 nm, most preferred 520 to 580 nm and their use for the preparation of inks, colorants, pigmented plastics for coatings, non-impact-printing material, color filters, cosmetics, polymeric ink particles, toners, dye lasers and electroluminescent devices. A luminescent device comprising a composition according to the present invention is high in the efficiency of electrical energy utilisation and high in luminance.

*Same Assignee as**10/576,914**See specification*



007501076B2

(12) **United States Patent**
Yamamoto et al.

US 7,501,076 B2
Patent: Mar. 10, 2009

(54) **FLUORESCENT
 DIKETOPYRROLOPYRROLES**

(75) Inventors: **Hiroshi Yamamoto**, Nishinomiya (JP);
Norihisa Dan, Yawata (JP)

(73) Assignee: **Ciba Specialty Chemicals
 Corporation**, Tarrytown, NY (US)

(*) Notice: Subject to any disclaimer, the term of this
 patent is extended or adjusted under 35
 U.S.C. 154(b) by 86 days.

(21) Appl. No.: **10/551,976**

(22) PCT Filed: **Apr. 1, 2004**

(86) PCT No.: **PCT/EP2004/050403**

§ 371 (c)(1).

(2), (4) Date: **Jul. 13, 2006**

(87) PCT Pub. No.: **WO2004/090046**

PCT Pub. Date: **Oct. 21, 2004**

(65) **Prior Publication Data**

US 2007/0010672 A1 Jan. 11, 2007

(30) **Foreign Application Priority Data**

Apr. 10, 2003 (EP) 03100972

(51) **Int. Cl.**

C09K 11/06 (2006.01)

B32B 9/00 (2006.01)

C07D 401/14 (2006.01)

(52) **U.S. Cl.** **252/301.16**; 252/301.26;
 428/690; 428/917; 546/256; 546/276.7

(58) **Field of Classification Search** 548/453;
 252/301.16, 301.26; 313/504, 506; 428/690,
 428/917; 544/333; 546/256, 276.7

See application file for complete search history.

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 2004/0180235 A1 9/2004 Yamamoto et al. 428/690
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 EP 1 078 970 2/2001
 EP 1 087 005 3/2001
 EP 1 087 006 3/2001
 EP 1087005 A1 * 3/2001
 EP 1087006 A1 * 3/2001
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 Patent abstracts of Japan vol. 018, No. 145 (C-1178; of JP 05320633).
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 English Language abstract No. 2002-210368[27] of JP 2001257077.
 English Language abstract No. 2002-210369[27] of JP 2001257078.

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Primary Examiner—Kamal A Saeed

Assistant Examiner—Kristin Bianchi

(74) *Attorney, Agent, or Firm*—Joseph C. Suhadolnik

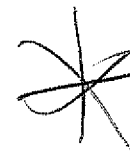
(57) **ABSTRACT**

The present invention relates to fluorescent diketopyrrolopyrrole of the formula (I), a process for their preparation and their use for the preparation of inks, colorants, pigmented plastics for coatings, non-impact-printing material, color filters, cosmetics, polymeric ink particles, toners, as fluorescent tracers, in color changing media, in solid dye lasers and electroluminescent devices. A luminescent device comprising a composition according to the present invention is high in the efficiency of electrical energy utilisation and high in luminance.

12 Claims, No Drawings



US005808094A

**United States Patent** [19][11] **Patent Number:** **5,808,094****Mizuguchi et al.**[45] **Date of Patent:** **Sep. 15, 1998****[54] PREPARATION OF MIXED CRYSTALS AND SOLID SOLUTIONS OF 1,4-DIKETOPYRROLOPYRROLES**

[75] Inventors: **Jin Mizuguchi**, Yokohama, Japan;
Zhimin Hao; **Olof Wallquist**, both of
 Marly, Switzerland; **Abul Iqbal**,
 Arconciel, Switzerland

[73] Assignee: **Ciba Specialty Chemicals Corporation**, Tarrytown, N.Y.

[21] Appl. No.: **898,140**[22] Filed: **Jul. 22, 1997****Related U.S. Application Data**

[62] Division of Ser. No. 712,721, Sep. 12, 1996, Pat. No. 5,693,824.

[30] Foreign Application Priority Data

Sep. 20, 1995 [CH] Switzerland 2651/95

[51] Int. Cl.⁶ **C07D 487/04**; C07D 209/02;
 C07D 405/14; C07D 409/14

[52] U.S. Cl. **548/453**; 548/454; 548/465;
 548/466; 548/467; 548/515; 544/242; 544/333;
 544/335; 546/251; 546/276.7; 546/278.4;
 549/1; 549/29; 549/59; 549/74; 549/78;
 549/200; 549/491; 549/497; 106/287.21;
 106/401; 106/496; 106/498

[58] Field of Search 548/453, 454,
 548/465, 512, 515; 106/287.21, 401, 496,
 498

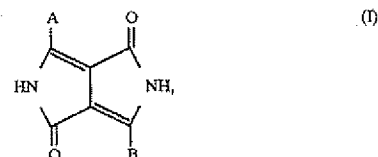
[56] References Cited**U.S. PATENT DOCUMENTS**

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Primary Examiner—Johann Richter
 Assistant Examiner—Jane C. Oswecki
 Attorney, Agent, or Firm—Kevin T. Mansfield

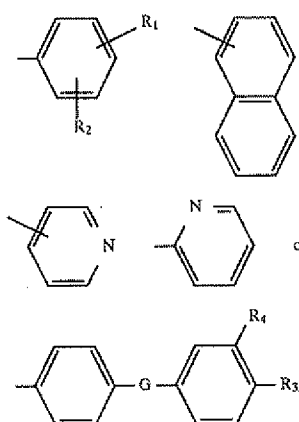
[57] ABSTRACT

A process for the preparation of mixed crystals of 1,4-diketopyrrolo[3,4-c]pyrroles, consisting of 1 mol each of two different compounds of formula



by heating a corresponding mixture in solid form to the temperature range from 220° to 380° C.

A and B are, for example, each a group of formula



wherein

R₁ and R₂ are each independently hydrogen, chloro, bromo, C₁-C₄alkyl, C₁-C₆alkoxy, C₁-C₆alkylamino, phenyl or —CN,

G is —O—, —NR₇—, —N=N— or —SO₂—,

R₃ and R₄ are hydrogen, and R₇ is hydrogen, methyl or ethyl.

The mixed crystals and solid solutions obtained are excellently suited for pigmenting high molecular weight material.

11 Claims, No Drawings

10/576,914

8/25/09

STN



L35 ANSWER 15 OF 64 COPYRIGHT ACS on STN

ACCESSION NUMBER: 2004:510462 HCAPLUS

DOCUMENT NUMBER: 141:61865

TITLE: **Diketopyrrolo[3,4-c]pyrroles and their organic electroluminescent devices showing good durability**

INVENTOR(S): Yauchi, Hiroyuki; Onikubo, Shunichi

PATENT ASSIGNEE(S): Toyo Ink Mfg. Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 21 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004175674	A	20040624	JP 2002-340206	20021125 <--
PRIORITY APPLN. INFO.:			JP 2002-340206	20021125 <--

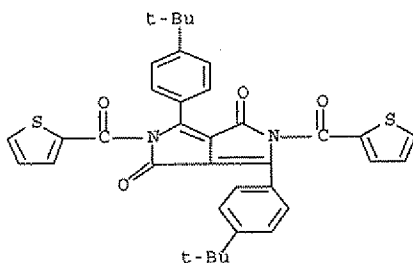
AB The pyrroles are I (A, B = electron-withdrawing group; R1, R2 = alkyl, aryl, heterocyclyl). The devices emit light from yellow to red with high intensity.

IT 96159-03-4P 709014-74-4P

RL: DEV (Device component use); IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (diketopyrrolopyrroles for organic electroluminescent devices emitting light from yellow to red)

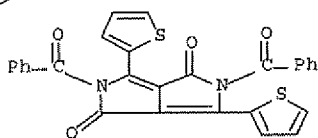
RN 709014-74-4 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 3,6-bis[4-(1,1-dimethylethyl)phenyl]-2,5-dihydro-2,5-bis(2-thienylcarbonyl)- (CA INDEX NAME)



RN 709014-77-7 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dibenzoyl-2,5-dihydro-3,6-di-2-thienyl- (CA INDEX NAME)



ST diketopyrrolopyrrole org electroluminescent device yellow red; phenyl benzoyl diketopyrrolopyrrole org electroluminescent device

IT Luminescent substances

(electroluminescent; diketopyrrolopyrroles for organic electroluminescent devices emitting light from yellow to red)

IT Electroluminescent devices

(organic; diketopyrrolopyrroles for organic electroluminescent devices emitting light from yellow to red)



L35 ANSWER 21 OF 64 COPYRIGHT ACS on STN

ACCESSION NUMBER: 2003:610553 HCAPLUS

DOCUMENT NUMBER: 139:171084

TITLE: **Fluorescent compositions comprising diketopyrrolopyrroles and electroluminescent devices employing the compositions**

INVENTOR(S): Yamamoto, Hiroshi; Dan, Norihisa

PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.

SOURCE: PCT Int. Appl., 61 pp.

DOCUMENT TYPE: Patent

LANGUAGE: English

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003064558	A1	20030807	WO 2003-EP650	20030123 <--
CA 2469269	A1	20030807	CA 2003-2469269	20030123 <--
AU 2003239272	A1	20030902	AU 2003-239272	20030123 <--
EP 1478713	A1	20041124	EP 2003-734603	20030123 <--
BR 2003007402	A	20041228	BR 2003-7402	20030123 <--
CN 1625589	A	20050608	CN 2003-803137	20030123 <--
JP 2005526152	T	20050902	JP 2003-564157	20030123 <--
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MX 2004006662	A	20041004	MX 2004-6662	20040708 <--
US 20050008892	A1	20050113	US 2004-501573	20040713 <--
IN 2004CN01907	A	20070921	IN 2004-CN1907	20040826 <--
PRIORITY APPLN. INFO.:				
				EP 2002-405067 A 20020201 <--
				EP 2002-405796 A 20020912 <--
				WO 2003-EP650 W 20030123 <--

AB **Fluorescent** compns. are described which comprise a guest chromophore and a host chromophore, where the absorption spectrum of the guest chromophore overlaps with the **fluorescence** emission spectrum of the host chromophore, where the host chromophore is a **diketopyrrolopyrrole** having a **photoluminescence** emission peak at 500 to 720 nm, preferably 500 to 600 nm, most preferred 520 to 580 nm and where the guest chromophore is a **diketopyrrolopyrrole** having an absorption peak at 500 to 720 nm, preferably 500 to 600 nm, most preferred 520 to 580 nm. **Electroluminescent** devices employing the compns. according to the present invention are also discussed.

IT **575451-78-4P 575451-79-5P 575451-80-8P 575451-83-1P**

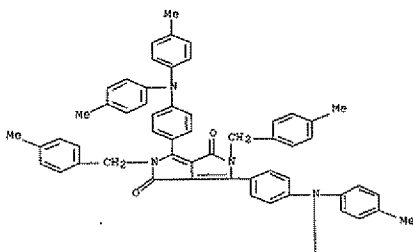
RL: DEV (Device component use); MOA (Modifier or additive use); PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

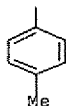
(**fluorescent** compns. comprising **diketopyrrolopyrroles** and **electroluminescent** devices employing the compns.)

RN 575451-78-4 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 3,6-bis[4-[bis(4-methylphenyl)amino]phenyl]-2,5-dihydro-2,5-bis[(4-methylphenyl)methyl]-

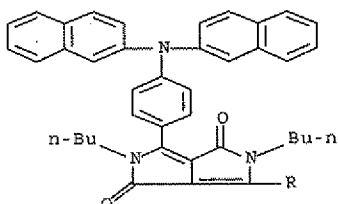
PAGE 1-A



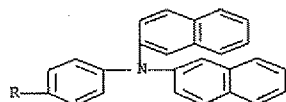


RN 575451-79-5 HCAPLUS
 CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dibutyl-3,6-bis[4-(di-2-naphthalenylamino)phenyl]-2,5-dihydro- (CA INDEX NAME)

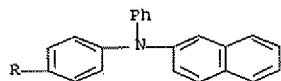
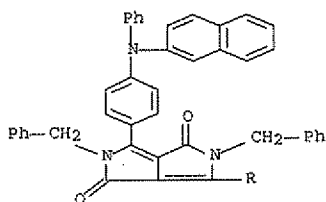
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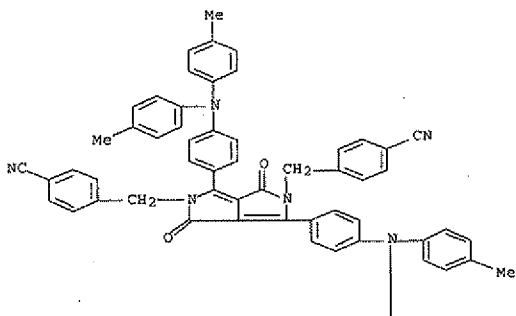


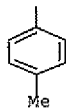
RN 575451-80-8 HCAPLUS
 CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dihydro-3,6-bis[4-(2-naphthalenylphenylamino)phenyl]-2,5-bis(phenylmethyl)- (CA INDEX NAME)



RN 575451-83-1 HCAPLUS
 CN Benzonitrile, 4,4'-[[3,6-bis[4-[bis(4-methylphenyl)amino]phenyl]-1,4-dioxopyrrolo[3,4-c]pyrrole-2,5(1H,4H)-diyl]bis(methylene)]bis- (9CI) (CA INDEX NAME)

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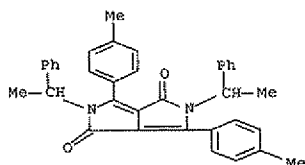
IT 575451-54-6P 575451-55-7P 575451-59-1P
 575451-60-4P 575451-61-5P 575451-62-6P
 575451-63-7P 575451-64-8P 575451-65-9P
 575451-67-1P 575451-68-2P 575451-69-3P
 575451-84-2P 575451-85-3P

RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(fluorescent compns. comprising diketopyrrolopyrroles and electroluminescent devices employing the compns.)

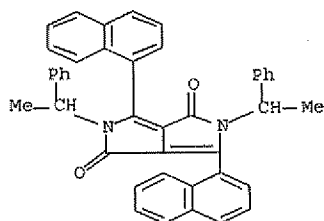
RN 575451-54-6 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dihydro-3,6-bis(4-methylphenyl)-2,5-bis(1-phenylethyl)- (CA INDEX NAME)



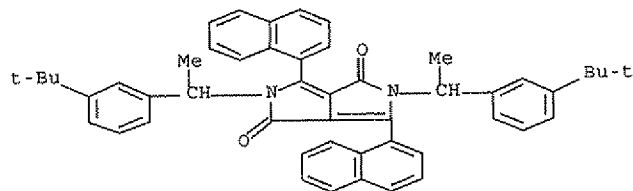
RN 575451-55-7 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dihydro-3,6-di-1-naphthalenyl-2,5-bis(1-phenylethyl)- (CA INDEX NAME)



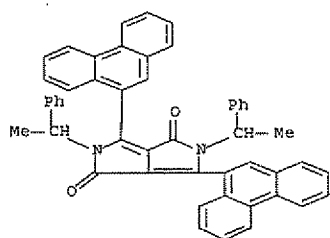
RN 575451-59-1 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-bis[1-[3-(1,1-dimethylethyl)phenyl]ethyl]-2,5-dihydro-3,6-di-1-naphthalenyl- (CA INDEX NAME)



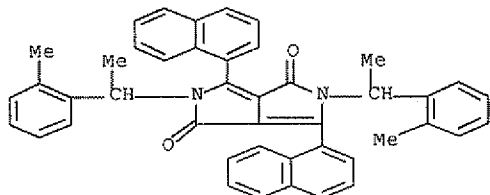
RN 575451-68-2 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dihydro-3,6-di-9-phenanthrenyl-2,5-bis(1-phenylethyl)- (CA INDEX NAME)



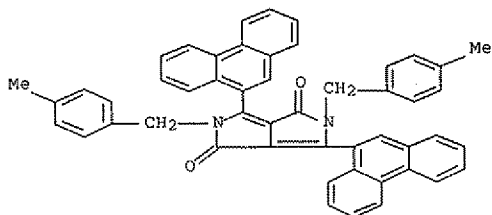
RN 575451-69-3 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dihydro-2,5-bis[1-(2-methylphenyl)ethyl]-3,6-di-1-naphthalenyl- (CA INDEX NAME)



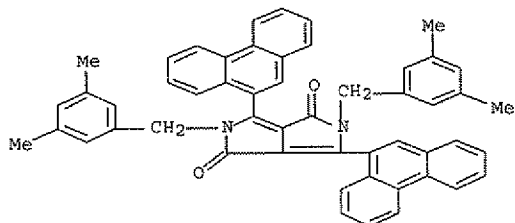
RN 361196-18-1 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dihydro-2,5-bis[(4-methylphenyl)methyl]-3,6-di-9-phenanthrenyl- (CA INDEX NAME)



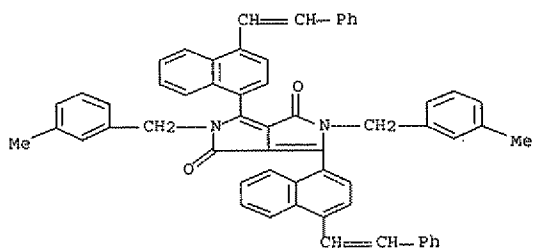
RN 482373-47-7 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-bis[(3,5-dimethylphenyl)methyl]-3,6-di-9-phenanthrenyl- (CA INDEX NAME)



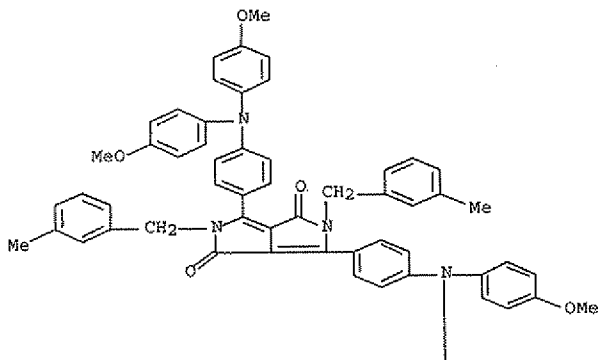
RN 575451-56-8 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dihydro-2,5-bis[(3-methylphenyl)methyl]-3,6-bis[4-(2-phenylethenyl)-1-naphthalenyl]- (CA INDEX NAME)

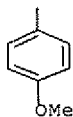


RN 575451-82-0 HCAPLUS
 CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 3,6-bis[4-[bis(4-methoxyphenyl)amino]phenyl]-2,5-dihydro-2,5-bis[(3-methylphenyl)methyl]-(CA INDEX NAME)

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IC ICM C09K011-06
 ICS H05B033-14; H01L051-20; C07D487-04
 ST fluorescent compn diketopyrrolopyrrole
 electroluminescent device
 IT Chromophores
 Electroluminescent devices
 Fluorescent substances
 (fluorescent compns. comprising diketopyrrolopyrroles
 and electroluminescent devices employing the compns.)
 IT 9011-14-7, PMMA
 RL: PRP (Properties); TEM (Technical or engineered material use); USES
 (Uses)
 (diketopyrrolopyrrole-doped color changing film;
 fluorescent compns. comprising diketopyrrolopyrroles
 and electroluminescent devices employing the compns.)
 IT 2085-33-8, Aluminum tris(8-hydroxyquinolinato)
 RL: DEV (Device component use); USES (Uses)
 (electron-transporting layer; fluorescent compns. comprising
 diketopyrrolopyrroles and electroluminescent devices
 employing the compns.)
 IT 575451-78-4P 575451-79-5P 575451-80-8P
 575451-83-1P
 RL: DEV (Device component use); MOA (Modifier or additive use); PRP
 (Properties); SPN (Synthetic preparation); TEM (Technical or engineered
 material use); PREP (Preparation); USES (Uses)
 (fluorescent compns. comprising diketopyrrolopyrroles
 and electroluminescent devices employing the compns.)
 IT 331687-86-6
 RL: DEV (Device component use); MOA (Modifier or additive use); PRP
 (Properties); TEM (Technical or engineered material use); USES (Uses)
 (fluorescent compns. comprising diketopyrrolopyrroles
 and electroluminescent devices employing the compns.)

10/576,914

8/25/09

STN



L35 ANSWER 27 OF 64 COPYRIGHT ACS on STN
 ACCESSION NUMBER: 2002:831834 HCAPLUS
 TITLE: Pyrromethene metal complexes and light emitting device composition and light emitting devices using the same
 INVENTOR(S): Murase, Seiichiro; Tominaga, Tsuyoshi; Kohama, Akira
 PATENT ASSIGNEE(S): Toray Industries, Inc., Japan
 SOURCE: Eur. Pat. Appl., 54 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: English

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1253151	A1	20021030	EP 2002-252947	20020425 <--
EP 1253151	B1	20050112		
TW 565604	B	20031211	TW 2002-91107585	20020415 <--
JP 2003012676	A	20030115	JP 2002-117229	20020419 <--
JP 4000893	B2	20071031		
US 20030082406	A1	20030501	US 2002-126652	20020422 <--
US 6805978	B2	20041019		
SG 121713	A1	20060526	SG 2002-2483	20020424 <--
KR 856981	B1	20080904	KR 2002-22535	20020424 <--
CN 1390841	A	20030115	CN 2002-124569	20020425 <--
AT 286903	T	20050115	AT 2002-252947	20020425 <--
CN 1690162	A	20051102	CN 2005-10071206	20020425 <--
CN 1308414	C	20070404		
CN 101393970	A	20090325	CN 2008-10166054	20020425 <--
JP 2003086379	A	20030320	JP 2002-150546	20020524 <--
JP 4061969	B2	20080319		

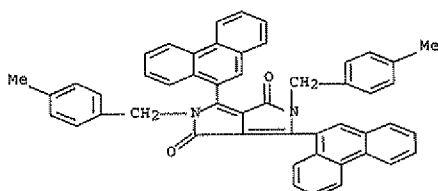
PRIORITY APPLN. INFO.:

JP 2001-127311	A	20010425 <--
JP 2001-158325	A	20010528 <--
KR 2002-22535	A3	20020424 <--
CN 2002-124569	A3	20020425 <--

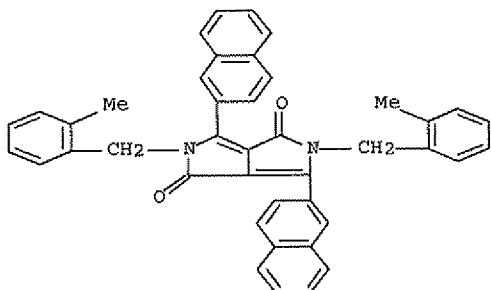
AB Pyrromethene metal complexes are described by the general formula I (R1, R2, and each L = independently selected H, alkyl, cycloalkyl, aralkyl, alkenyl, cycloalkenyl, alkynyl, hydroxyl, mercapto, alkoxy, alkylthio, aryl ether, aryl thioether, aryl, heterocyclic, halogen, haloalkane, haloalkene, haloalkyne, cyano, aldehyde, carbonyl, carboxyl, ester, carbamoyl, amino, nitro, silyl, siloxanyl, and fused aromatic and alicyclic rings formed from Ar1-4 and L; M + a metal having a valence of m selected from boron, beryllium, magnesium, chromium, iron, nickel, copper, zinc, and platinum; and Ar1-5 = independently selected optionally substituted aryl groups with the proviso that any of Ar1-4, together with an adjacent group selected from R1, R2 and the or each group L may form a fused aromatic or alicyclic ring). **Light-emitting devices** comprising ≥ 1 of a **diketopyrrolo[3,4-c]pyrrole** derivative and an organic **fluorescent** material having a **fluorescent** peak wavelength in the range 580-720 nm; and a **light-emitting device** composition containing I are also described.

RN 361196-18-1 HCAPLUS

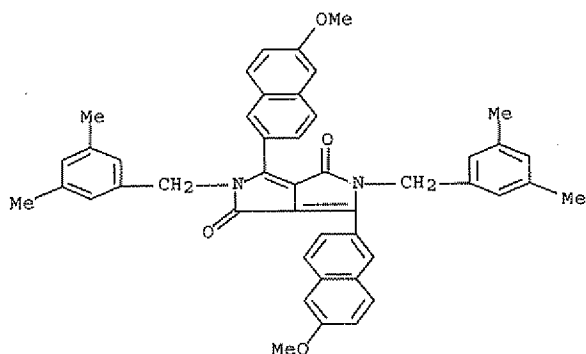
CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dihydro-2,5-bis[(4-methylphenyl)methyl]-3,6-di-9-phenanthrenyl- (CA INDEX NAME)



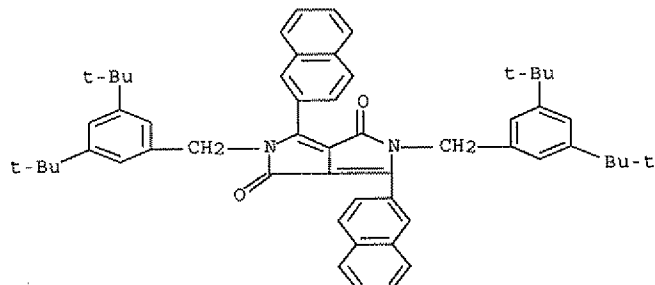
RN 474067-31-7 HCAPLUS
 CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dihydro-2,5-bis[(2-methylphenyl)methyl]-3,6-di-2-naphthalenyl- (CA INDEX NAME)



RN 474067-33-9 HCAPLUS
 CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-bis[(3,5-dimethylphenyl)methyl]-2,5-dihydro-3,6-bis(6-methoxy-2-naphthalenyl)- (CA INDEX NAME)



RN 474067-35-1 HCAPLUS
 CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-bis[[3,5-bis(1,1-dimethylethyl)phenyl]methyl]-2,5-dihydro-3,6-di-2-naphthalenyl- (CA INDEX NAME)



ST pyrromethene metal complex light emitting device compn
 IT Electroluminescent devices
 Luminescent substances
 (pyrromethene metal complexes and light-emitting
 device compns. and the devices)

L35 ANSWER 42 OF 64 COPYRIGHT ACS on STN

ACCESSION NUMBER: 2000:185714 HCAPLUS

TITLE: New **photoluminescent** conjugated polymers with 1,4-dioxo-3,6-diphenylpyrrolo[3,4-c]pyrrole (DPP) and 1,4-phenylene units in the main chain

AUTHOR(S): Beyerlein, Thomas; Tieke, Bernd

CORPORATE SOURCE: Institut für Physikalische Chemie der Universität zu

~~Köln, Köln, D-50939, Germany~~

SOURCE: Macromolecular Rapid Communications (2000), 21(4), 182-189

CODEN: MRCOE3; ISSN: 1022-1336

PUBLISHER: Wiley-VCH Verlag GmbH

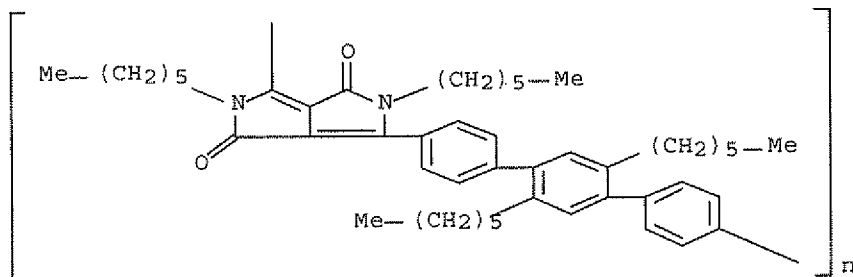
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Palladium-catalyzed aryl-aryl coupling reaction can be applied to prepare π -conjugated polymers with 1,4-dioxo-3,6-diphenylpyrrolo[3,4-c]pyrrole (DPP) and phenylene units in the backbone. These polymers are of orange color and showed a strong **photoluminescence**. The photochem. stability is higher than for corresponding saturated polymers containing isolated DPP units in the main chain. Good solubility and processability into thin films render the compds. suitable for electronic applications. The **polymers** show **electroluminescent** properties, the maximum **emission** occurring at 627 nm.

RN 266357-56-6 HCAPLUS

CN Poly[(2,5-dihexyl-2,3,5,6-tetrahydro-3,6-dioxopyrrolo[3,4-c]pyrrole-1,4-diyl)(2',5'-dihexyl[1,1':4',1''-terphenyl]-4,4''-diyl)] (9CI) (CA INDEX NAME)



ST **photoluminescent** conjugated polymer
dioxodiphenylpyrrolopyrrole phenylene; **electroluminescent**
 conjugated **polymer dioxodiphenylpyrrolopyrrole**
 phenylene

IT **Luminescence****Luminescence, electroluminescence**

(preparation and properties of **photoluminescent** conjugated
 polymers with **dioxodiphenylpyrrolopyrrole** and phenylene units
 in main chain)

IT 266357-54-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation and polymerization of)

IT 266357-55-5P 266357-56-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and properties of **photoluminescent**)

10/576,914

8/25/09

STN

L35 ANSWER 50 OF 64 COPYRIGHT ACS on STN

ACCESSION NUMBER: 1997:553163 HCAPLUS

DOCUMENT NUMBER: 127:191921

ORIGINAL REFERENCE NO.: 127:37215a,37218a

TITLE: Polymerizable diketo **pyrrolopyrroles**, their preparation and (co)polymerization

INVENTOR(S): Eldin, Sameer Hosam; Iqbal, Abul; Hao, Zhimin; Lamatseh, Bernd

PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.

SOURCE: Eur. Pat. Appl., 28 pp.

CODEN: EPXXDW

DOCUMENT TYPE: **Patent**

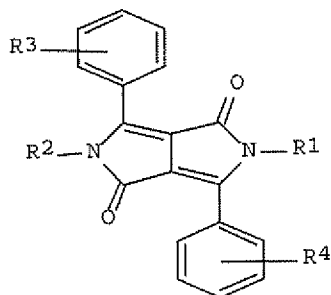
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 787730	A1	19970806	EP 1997-810030	19970122 <--
EP 787730	B1	20010801		
CA 2196139	A1	19970731	CA 1997-2196139	19970128 <--
TW 442505	B	20010623	TW 1997-86100902	19970128 <--
CN 1165824	A	19971126	CN 1997-102513	19970129 <--
US 5750723	A	19980512	US 1997-789895	19970129 <--
JP 09323993	A	19971216	JP 1997-16468	19970130 <--
			CH 1996-228	A 19960130 <--

PRIORITY APPLN. INFO.:



AB The polymerizable dyes, which can be incorporated in or grafted to polymers to be colored, have the structure I (R1, R2 = H, C12-24 alkyl, C6-24 alkyl interrupted by ≥ 1 O or S, CO2R5; R3 = polymerizable group; R4 = H, halo, Me, OMe, CN, Ph, R3, C6-24 alkyl or alkoxy or alkylthio optionally interrupted by ≥ 1 O or S; R5 = C4-18 alkyl, C5-10 cycloalkyl). Thus, p-methoxybenzonitrile was cyclocondensed with diisopropyl succinate to give I (R1 = R2 = H, R3 = R4 = 4-OMe), which was alkylated with 2 mol Br(CH2CH2O)2Et and hydrolyzed in CH2Cl2 in the presence of BBr3 to give I [R1 = R2 = (CH2CH2O)2Et, R3 = R4 = 4-OH] (II). II was copolymd. with hexamethylene diisocyanate to give an orange-red polyurethane.

IT 194029-85-1P 194029-87-3P 194295-76-6P

RL: IMF (Industrial manufacture); PREP (Preparation)

(preparation and polymerization of **pyrrolopyrroledione** dyes to colored polymers)ST **pyrrolopyrroledione** dye polymerizable

IT Dyes

(preparation of polymerizable **pyrrolopyrroledione** dyes)

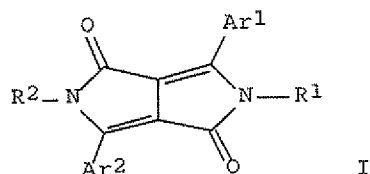
10/576,914

8/25/09

STN

L35 ANSWER 37 OF 64 COPYRIGHT ACS on STN
 ACCESSION NUMBER: 2001:228313 HCAPLUS
 DOCUMENT NUMBER: 134:273272
 TITLE: **Fluorescent diketopyrrolopyrroles**
 INVENTOR(S): Moretti, Robert; Hao, Zhimin; Yamamoto, Hiroshi
 PATENT ASSIGNEE(S): **Ciba Specialty Chemicals Holding Inc., Switz.**
 SOURCE: Eur. Pat. Appl., 28 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: **Patent**
 LANGUAGE: English

PATENT-NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1087005	A1	20010328	EP 2000-810847	20000919 <--
EP 1087005	B1	20040225		
TW 261064	B	20060901	TW 2000-89118230	20000906 <--
US 6603020	B1	20030805	US 2000-735080	20000907 <--
JP 2001097975	A	20010410	JP 2000-288313	20000922 <--
KR 753348	B1	20070830	KR 2000-56659	20000927 <--
US 20030187106	A1	20031002	US 2003-354602	20030130 <--
PRIORITY APPLN. INFO.:			EP 1999-810867	A 19990927 <--
			US 2000-735080	A3 20000907 <--



AB **Fluorescent diketopyrrolopyrrole** derivs. are described by the general formula I (Ar1, Ar2 = independently selected (un)substituted cyclic groups; R1, R2 = independently selected (un)substituted alkyl or allyl groups). Methods for preparing the derivs. are described which entail treating a precursor **diketopyrrolopyrrole** derivative are also described. A method of coloring high mol. weight organic materials (e.g., a polyamide, a polystyrene, preferably high impact polystyrene, polymethylmethacrylate or an ABS copolymer) by incorporating the derivs., as well as colored compns. incorporating the derivs. along with high mol. weight organic materials are also described. The use of the **diketopyrrolopyrrole** derivs. for the preparation of inks, colorants, pigmented plastics for coatings, non-impact-printing material, color filters, cosmetics, or for the preparation of polymeric ink particles, toners, dye lasers, and **electroluminescent** devices is also described.

L35 ANSWER 36 OF 64 COPYRIGHT ACS on STN

ACCESSION NUMBER: 2001:228314 HCAPLUS

DOCUMENT NUMBER: 134:273302

TITLE: **Electroluminescent devices comprising diketopyrrolopyrroles**

INVENTOR(S): Otani, Junji; Yamamoto, Hiroshi; Dan, Norihisa; Iqbal, Abul; Moretti, Robert

PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.

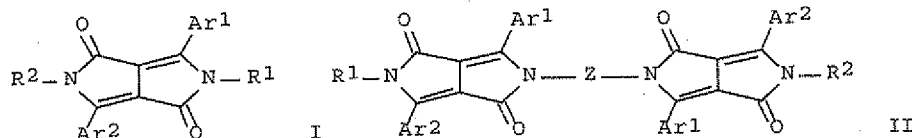
SOURCE: Eur. Pat. Appl., 44 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1087006	A1	20010328	EP 2000-810848	20000919 <--
EP 1087006	B1	20031015		
TW 503255	B	20020921	TW 2000-89117516	20000829 <--
US 7060843	B1	20060613	US 2000-657738	20000908 <--
EP 1329493	A2	20030723	EP 2003-9036	20000919 <--
EP 1329493	A3	20070523		
R: CH, DE, FR, GB, IT, LI				
JP 2001139940	A	20010522	JP 2000-288030	20000922 <--
JP 3854792	B2	20061206		
KR 803638	B1	20080219	KR 2000-56530	20000926 <--
US 20040009368	A1	20040115	US 2003-425201	20030429 <--
US 7001677	B2	20060221		
JP 2006319347	A	20061124	JP 2006-158476	20060607 <--
PRIORITY APPLN. INFO.:			EP 1999-810868	A 19990927 <--
			US 2000-657738	A3 20000908 <--
			EP 2000-810848	A3 20000919 <--
			JP 2000-288030	A3 20000922 <--



AB **Electroluminescent devices** are described which employ **fluorescent diketopyrrolopyrrole** derivs. described by the general formulas I and II (Ar1, Ar2 = independently selected (un)substituted cyclic groups; R1, R2 = independently selected (un)substituted alkyl or allyl groups; and Z = a diradical selected from a single bond, C2-6 alkylene, which can be substituted one to three times with C1-4 alkyl, C1-4 alkoxy, or Ph, phenylene, or naphthylene) in the **light-emitting layers**. The **fluorescent diketopyrrolopyrrole** derivs. are also claimed. Methods for preparing the derivs. are described which entail treating a precursor **diketopyrrolopyrrole** derivative are also described. A method of coloring high mol. weight organic materials (e.g., a polyamide, a polystyrene, preferably high impact polystyrene, polymethylmethacrylate or an ABS copolymer) by incorporating the derivs., as well as colored comps. incorporating the derivs. along with high mol. weight organic materials are also described.

IT 331687-86-6

RL: DEV (Device component use); USES (Uses)

(electroluminescent devices comprising

diketopyrrolopyrrole derivs. and the derivs. and their preparation)

10/576,914

8/25/09

STN

L35 ANSWER 6 OF 64 COPYRIGHT ACS on STN

ACCESSION NUMBER: 2005:235266 HCAPLUS

DOCUMENT NUMBER: 142:306146

TITLE: **Electroluminescent materials containing styryl compounds and diketopyrrolopyrroles, and red-emitting organic electroluminescent devices using them**

INVENTOR(S): Suda, Yasumasa; Toba, Yasumasa; Tanaka, Hiroaki; Amano, Saneomi

PATENT ASSIGNEE(S): Toyo Ink Mfg. Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 65 pp.

CODEN: JKXXAF

DOCUMENT TYPE: **Patent**

LANGUAGE: Japanese

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005068376	A	20050317	JP 2003-303555	20030827 <--

PRIORITY APPLN. INFO.: JP 2003-303555 20030827 <--

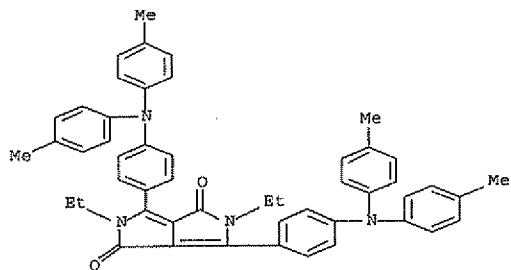
AB The materials contain styryl compds. I or II (R3-R10 = aliphatic hydrocarbyl, aromatic hydrocarbyl, aliphatic heterocyclyl, aromatic heterocyclyl; X1-X3 = aromatic heterocyclylene; R3R22, R4R24, R5R31, R6R33, R7R34, R8R36, R9R45, and R10R47 may form ring), and **diketopyrrolopyrroles** III [R11-R16 = H, aliphatic hydrocarbyl, aromatic hydrocarbyl, aliphatic heterocyclyl, aromatic heterocyclyl; X4, X5 = O, (un)substituted imino, (un)substituted CH2]. Thus, an **organic electroluminescent device** having an **emitter layer** containing I (R3 = R4 = R5 = R6 = OMe, X1 = 2,5-dicyano-1,4-phenylene, other = H) and III (R11 = R12 = R13 = R14 = 4-MeOC6H4, R15 = R16 = H, Ar1 = Ar2 = 1,4-phenylene, X4 = X5 = O) showed high **luminescence** intensity and color purity at low operation voltage, and lengthened service life.

IT 488134-89-0 536761-83-8 847947-24-4

RL: DEV (Device component use); MOA (Modifier or additive use); USES (dopant; **electroluminescent materials containing styryl compds. and diketopyrrolopyrroles for red-emitting organic electroluminescent devices**)

RN 488134-89-0 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 3,6-bis[4-[bis(4-methylphenyl)amino]phenyl]-2,5-diethyl-2,5-dihydro- (CA INDEX NAME)



ST **diketopyrrolopyrrole styryl compd red emitting org electroluminescent device**

IT **Luminescent substances**
(**electroluminescent; electroluminescent materials containing styryl compds. and diketopyrrolopyrroles for red-emitting organic electroluminescent devices**)

IT **Electroluminescent devices**
(**red-emitting; electroluminescent materials containing styryl compds. and diketopyrrolopyrroles for red-emitting organic electroluminescent devices**)



US005821373A

United States Patent [19]**Hao et al.**[11] **Patent Number:** **5,821,373**[45] **Date of Patent:** **Oct. 13, 1998**[54] **SOLID SOLUTIONS OF 1,4-DIKETOPYRROLOPYRROLES**[75] Inventors: **Zhimin Hao; Olof Wallquist**, both of Marly, Switzerland[73] Assignee: **Ciba Specialty Chemicals Corporation**, Tarrytown, N.Y.[21] Appl. No.: **712,722**[22] Filed: **Sep. 12, 1996**[30] **Foreign Application Priority Data**

Sep. 18, 1995 [CH] Switzerland 2630/95

[51] Int. Cl.⁶ **C07D 487/04; C09B 48/00; C08K 5/07; C08K 5/3415**[52] U.S. Cl. **548/453; 548/215; 548/240; 548/255; 548/266.4; 548/335.1; 548/343.5; 548/364.7; 548/513; 548/515; 549/59; 549/472; 546/56; 546/208; 544/111; 544/373; 106/498; 534/558; 534/561; 534/816; 534/885**[58] Field of Search **548/453; 106/498**

[56]

References Cited**U.S. PATENT DOCUMENTS**

4,579,949	4/1986	Rochat et al.	546/167
4,720,305	1/1988	Iqbal et al.	106/288
4,783,540	11/1988	Babler	548/453
4,810,304	3/1989	Jaffe et al.	106/494
5,476,949	12/1995	Wallquist et al.	548/453
5,518,539	5/1996	Hao et al.	106/495
5,554,217	9/1996	Babler	106/494
5,565,578	10/1996	Babler	548/453
5,641,351	6/1997	Babler	106/495
5,708,188	1/1998	Hao et al.	548/453

Primary Examiner—Johann Richter*Assistant Examiner*—Jane C. Oswecki*Attorney, Agent, or Firm*—Kevin T. Mansfield

[57]

ABSTRACT

Solid solutions consisting of 3,6-bis(biphenyl-4-yl)- 2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione and either a) a second 1,4-diketopyrrolopyrrole or b) a quinacridone, which are further defined herein, are outstandingly suited to pigments high molecular weight organic material.

6 Claims, No Drawings



US006036766A

United States Patent [19]
Hendi et al.

[11] **Patent Number:** **6,036,766**
 [45] **Date of Patent:** ***Mar. 14, 2000**

[54] **MIXED CRYSTALS AND SOLID SOLUTIONS
 OF 1,4-DIKETOPYRROLOPYRROLES**

[58] **Field of Search** 548/453; 106/494;
 106/495, 497, 498

[75] **Inventors:** **Shivakumar Basalingappa Hendi,**
Newark; Fridolin Bähler, Hockessin,
both of Del.; Zhimin Hao, Marly; Abul
Iqbal, Arconciel, both of Switzerland

[56] **References Cited**

U.S. PATENT DOCUMENTS

[73] **Assignee:** **Ciba Specialty Chemicals**
Corporation, Tarrytown, N.Y.

4,579,949	4/1986	Rochat et al.	546/167
4,720,305	1/1988	Iqbal et al.	106/288
4,810,304	3/1989	Jaffe et al.	106/494
5,529,623	6/1996	Hendi et al.	106/495
5,565,578	10/1996	Bähler	548/453
5,756,746	5/1998	Hao et al.	546/56

[*] **Notice:** This patent issued on a continued prosecution application filed under 37 CFR 1.53(d), and is subject to the twenty year patent term provisions of 35 U.S.C. 154(a)(2).

Primary Examiner—Laura L. Stockton
Attorney, Agent, or Firm—Kevin T. Mansfield; David R. Crichton

[21] **Appl. No.:** **08/806,488**

[57] **ABSTRACT**

[22] **Filed:** **Feb. 27, 1997**

Related U.S. Application Data

[60] **Provisional application No.** 60/012,938, Mar. 6, 1996.

[51] **Int. Cl.⁷** **C08K 5/3415; C09B 48/00;**
C09B 67/22

[52] **U.S. Cl.** **106/494; 106/495; 106/497;**
106/498; 548/453

Ternary solid solutions useful as pigments are disclosed. The ternary solid solutions result from incorporating a third component, which is a diketopyrrolopyrrole or quinacridone pigment, into the crystal lattice of the mixed crystal formed from equimolar amounts of two different diketopyrrolopyrrole pigments.

21 Claims, No Drawings

10/576,914

8/25/09

STN

L35 ANSWER 55 OF 64 COPYRIGHT ACS on STN

ACCESSION NUMBER: 1995:763565 HCAPLUS

TITLE: 1,4-diketopyrrolo[3,4-c]pyrroles,
their preparation and their use

INVENTOR(S): Zambounis, John; Hao, Zhimin; Iqbal, Abul

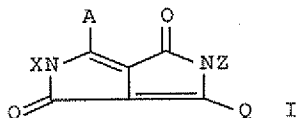
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.

SOURCE: Eur. Pat. Appl., 35 pp.

DOCUMENT TYPE: Patent

LANGUAGE: German

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 648770	A2	19950419	EP 1994-810580	19941004 <--
EP 648770	A3	19950531		
EP 648770	B1	20000517		
US 5484943	A	19960116	US 1994-319406	19941006 <--
CA 2117865	A1	19950414	CA 1994-2117865	19941011 <--
JP 07188234	A	19950725	JP 1994-246632	19941013 <--
JP 3596915	B2	20041202		
EP 690057	A1	19960103	EP 1995-810412	19950620 <--
EP 690057	B1	19990908		
EP 690058	A1	19960103	EP 1995-810413	19950620 <--
EP 690058	B1	19990908		
EP 690059	A1	19960103	EP 1995-810414	19950620 <--
EP 690059	B1	19990908		
US 5591865	A	19970107	US 1995-493853	19950622 <--
US 5646299	A	19970708	US 1995-493776	19950622 <--
US 5650520	A	19970722	US 1995-493516	19950622 <--
CA 2152744	A1	19951230	CA 1995-2152744	19950627 <--
CA 2152745	A1	19951230	CA 1995-2152745	19950627 <--
CA 2152748	A1	19951230	CA 1995-2152748	19950627 <--
JP 08020731	A	19960123	JP 1995-163153	19950629 <--
JP 3637105	B2	20050413		
JP 08027391	A	19960130	JP 1995-163151	19950629 <--
JP 3645314	B2	20050511		
JP 08048908	A	19960220	JP 1995-163152	19950629 <--
JP 3645315	B2	20050511		
US 5616725	A	19970401	US 1995-541004	19951011 <--
PRIORITY APPLN. INFO.:			CH 1993-3079	A 19931013 <--
			CH 1994-2074	A 19940629 <--
			CH 1994-2075	A 19940629 <--
			CH 1994-2076	A 19940629 <--
			US 1994-319406	A3 19941006 <--



AB The pyrrolopyrrolediones (I; A, Q = aromatic group; X = H, RO₂C; Z = CO₂R, where R = organic group) are obtained for use as UV- fluorescent pigments. Thus, 1,4-diketo-3,6- diphenylpyrrolo[3,4-c]pyrrole was treated with di-tert-Bu carbonate to give I (A = Q = Ph; X = Z= tert-butoxycarbonyl).

ST pyrrolopyrroledione fluorescent pigment

IT Luminescent substances

Recording materials

(preparation of diketopyrrolopyrrole fluorescent pigments)

10/576,914

8/25/09

STN

L35 ANSWER 58 OF 64 COPYRIGHT ACS on STN

ACCESSION NUMBER: 1993:671861 HCAPLUS

TITLE: Rational designs of multifunctional polymers

AUTHOR(S): Chan, Wai Kin; Chen, Yongming; Peng, Zhonghua; Yu, Luping

~~CORPORATE SOURCE: Dep. Chem., Univ. Chicago, Chicago, IL, 60637, USA~~SOURCE: Journal of the American Chemical Society (1993),
115(25), 11735-43

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

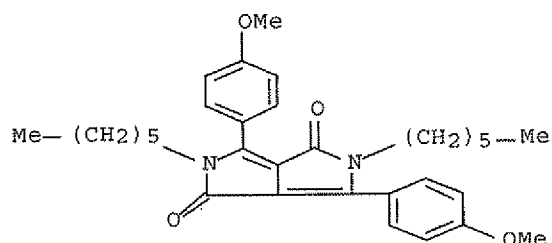
AB To manifest **photorefractive effects**, a polymer must possess a photocharge generator, a charge transporter, a charge trapping center, and a nonlinear optical (NLO) chromophore. The authors utilize the Stille coupling reaction to synthesize a novel type of multifunctional polymer that contains a conjugated backbone (with p-phenylene, 2,5- **thiophenediyl**, and **pyrrolo[3,4-c]pyrrole** -1,3-dione-3,6-diyl units) and a (stilbene group-containing) second-order NLO chromophore. The expectation that the polymers will possess photorefractivity (PR) is the design idea behind the structure of the polymers. Because the conjugated backbone absorbs photons in the visible region and is photoconductive, it is expected to play the triple role of charge generator, charge transporter, and backbone. Thus, the four functionalities necessary to manifest the PR effect exist simultaneously in a single polymer. Second harmonic generation and photocond. measurements reveal that the polymers are NLO active and photoconductive. Two beam-coupling expts. clearly indicate asym. optical energy exchange, which is an unambiguous demonstration of PR.

IT 151426-36-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and demethylation of)

RN 151426-36-7 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dihexyl-2,5-dihydro-3,6-bis(4-methoxyphenyl)- (CA INDEX NAME)



10/576,914

8/25/09

STN

L35 ANSWER 59 OF 64 COPYRIGHT ACS on STN

ACCESSION NUMBER: 1993:29594 HCAPLUS

TITLE: Organic electroluminescent element

INVENTOR(S): Matsumura, Michio; Kudo, Tetsu; Wooden, Gary

PATENT ASSIGNEE(S): Japat Ltd., Switz.

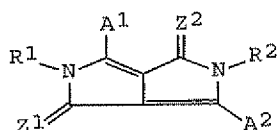
SOURCE: Eur. Pat. Appl., 22 pp.

CODEN: EPXXDW

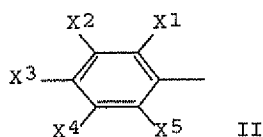
DOCUMENT TYPE: Patent

LANGUAGE: English

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 499011	A1	19920819	EP 1991-810097	19910212 <--
R: GB				
PRIORITY APPLN. INFO.:			EP 1991-810097	19910212 <--



I



II

AB Electroluminescent devices are described which employ as a light-emitting material compds. described by the general formula I (Z1 and Z2 are independently selected from O and S; R1 and R2 are independently selected from H, C1-18 alkyl groups, C3-18 alkenyl groups in which the double bond is not in the C1 position, or a phenylalkyl group with a C1-5 alkyl group; A1 and A2 are independently selected from 3-pyridyl, 4-pyridyl, or groups described by the general formula II in which X1 and X5 are independently selected from H, C1-5 alkyl groups, C1-5 alkoxy groups, or halogens, and X1, X3, and X4 are independently selected from H, C1-5 alkyl groups, C1-5 alkoxy groups, dialkylamino groups with 1-5 C/alkyl group, Ph, CN, -CF3, or halogens).

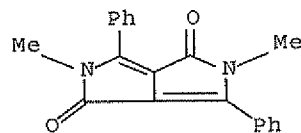
IT 96159-17-0 119273-55-1

RL: PRP (Properties)

(electroluminescent elements with light-emitting layers from)

RN 96159-17-0 HCAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dihydro-2,5-dimethyl-3,6-diphenyl- (CA INDEX NAME)



ST pyrrolopyrrole deriv electroluminescent device

IT Electroluminescent devices

(using pyrrolopyrrole derivs. as light-emitting layers)

IT 96159-17-0 119273-55-1

RL: PRP (Properties)

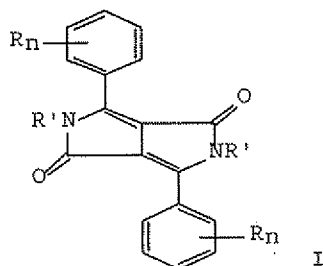
(electroluminescent elements with light-emitting layers from)

10/576,914

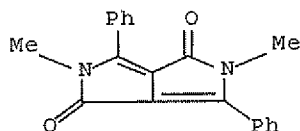
8/25/09

STN

L35 ANSWER 64 OF 64 COPYRIGHT ACS on STN
 ACCESSION NUMBER: 1987:460637 HCAPLUS
 TITLE: **Fluorescent dyes with large Stokes shifts - soluble dihydropyrrolopyrrolediones**
 AUTHOR(S): Potrawa, Thomas; Langhals, Heinz
 CORPORATE SOURCE: Inst. Org. Chem., Univ. Muenchen, Munich, D-8000/2, Fed. Rep. Ger.
 SOURCE: Chemische Berichte (1987), 120(7), 1075-8
 CODEN: CHBEAM; ISSN: 0009-2940
 DOCUMENT TYPE: Journal
 LANGUAGE: German



AB **Fluorescent 3,6-diaryl-2,5-dihydropyrrolo[3,4-c] pyrrole-1,4-diones (I; R' = H; R = Me, tert-Bu; n = 0-2) and 3,6-diaryl-2,5-dihydro-2,5-dimethylpyrrolo[3,4-c]pyrrole -1,4-diones (I; R' = Me; R = Me, tert-Bu; n = 0-2) were prepared from RnC6H4-nCN and di-Et succinate followed by optional methylation. I (R = tert-Bu) were photostable in organic solvents. If a conformational conversion followed the excitation, Stokes shifts of ≤70 nm with fluorescent quantum yields of ≤95% were obtained in CHCl3.**
 IT 96159-17-0P 107680-84-2P 107680-85-3P
 107711-05-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of **fluorescent**, Stokes shift in relation to)
 RN 96159-17-0 HCAPLUS
 CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-dihydro-2,5-dimethyl-3,6-diphenyl-
 (CA INDEX NAME)



CC 41-5 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)
 ST **pyrrolopyrroledione fluorescent dye; Stokes shift**
pyrrolopyrroledione dye
 IT **Fluorescence**
 (of **pyrrolopyrrolediones**, Stokes shift in relation to)
 IT Dyes
 (fluorescent, **pyrrolopyrrolediones**, preparation and Stokes shift of)